

EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	3	((("2882323") or ("5872277") or ("6278016"))).PN.	US-PGPUB; USPAT	OR	OFF	2007/05/30 12:48
L2	1	DE-3021414-\$.did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:49
L3	2	DE-3105399-\$.did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:51
L4	1	GB-1341015-\$.did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:51
L5	2	GB-2051067-\$.did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:52
L6	2	JP-60239443-\$.did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:52
L7	0	WO-2000026175-\$.did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:53
L8	1	WO-200026175-\$.did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:54
L9	1105	diene near3 carboxylic adj acid	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:54
L10	454	I9 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 12:55
L11	363	myrcene near5 isoprene	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 12:56
L12	257	I11 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 12:56

EAST Search History

L13	399	myrcene near5 isoprene	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:56
L14	257	l13 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:07
L15	0	l10 and l14	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:03
L16	18353	"alkanoic acids"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:06
L17	605	"alkanoic acids".ti.	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:08
L18	268	l17 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:08
L19	0	l14 and l18	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/05/30 13:07
L20	2636	"alkanoic acids".ti.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/05/30 13:08
L21	268	l20 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:09
L22	1	l21 and myrcene	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:09
L23	109	ester near5 diene adj compound	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/05/30 13:09
L24	67	l23 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:10
S1	239	"560/249".CCLS.	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 10:30

EAST Search History

S2	21	((JAMES) near2 (BABLER)).INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/29 14:58
S3	3	((JAMES) near2 (BABLER)).INV.	EPO; JPO; DERWENT	OR	ON	2007/05/29 14:58
S4	239	"560/249".CCLS.	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/29 15:01
S5	61	S4 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 12:55
S6	1	("5872277").PN.	US-PGPUB; USPAT	OR	OFF	2007/05/30 10:30
S7	1	("5872277").URPN.	USPAT	OR	ON	2007/05/30 11:44
S8	0	GB-1172516-\$.did.	USPAT	OR	ON	2007/05/30 11:45
S9	0	GB-1172516-\$.did.	US-PGPUB; USPAT; USOCR; EPO	OR	ON	2007/05/30 12:47

SEARCH HISTORY

=> d his nofile

(FILE 'HOME' ENTERED AT 10:23:49 ON 16 MAY 2007)

FILE 'HCAPLUS' ENTERED AT 10:24:09 ON 16 MAY 2007

E US20070055076/PN

L1 1 SEA ABB=ON PLU=ON US20070055076/PN
D ALL
SEL RN

FILE 'REGISTRY' ENTERED AT 10:25:28 ON 16 MAY 2007

L2 35 SEA ABB=ON PLU=ON (100-66-3/BI OR 105-87-3/BI OR
105-90-8/BI OR 105-91-9/BI OR 106-24-1/BI OR 106-25-2/B
I OR 106-42-3/BI OR 107-92-6/BI OR 108-21-4/BI OR
108-88-3/BI OR 108-90-7/BI OR 108-94-1/BI OR 109-20-6/B
I OR 1191-16-8/BI OR 123-35-3/BI OR 123-86-4/BI OR
127-08-2/BI OR 127-09-3/BI OR 137-40-6/BI OR 138-86-3/B
I OR 141-12-8/BI OR 142-96-1/BI OR 157258-67-8/BI OR
19559-59-2/BI OR 3915-83-1/BI OR 503-74-2/BI OR
5392-40-5/BI OR 556-82-1/BI OR 64-19-7/BI OR 78-79-5/BI
OR 78-93-3/BI OR 79-09-4/BI OR 79-31-2/BI OR 80-26-2/B
I OR 851785-97-2/BI)

L3 19 SEA ABB=ON PLU=ON L2 AND ?ACID?/CNS
D SCAN

L4 1 SEA ABB=ON PLU=ON 123-35-3/RN
D SCAN
D IDE

L5 1 SEA ABB=ON PLU=ON 78-79-5/RN
D SCAN
D IDE

L6 1 SEA ABB=ON PLU=ON 1191-16-8/RN
D SCAN
D CN
D IDE

L7 1 SEA ABB=ON PLU=ON 105-87-3/RN
D SCAN
D IDE

L8 1 SEA ABB=ON PLU=ON 141-12-8/RN
D IDE

L9 11 SEA ABB=ON PLU=ON L2 AND ?ACETATE?/CNS

FILE 'STNGUIDE' ENTERED AT 10:44:21 ON 16 MAY 2007

FILE 'CASREACT' ENTERED AT 10:50:09 ON 16 MAY 2007

L10 1 SEA ABB=ON PLU=ON 123-35-3/RCT(L) (105-87-3/PRO OR
141-12-8/PRO)
D SCAN

L11 2 SEA ABB=ON PLU=ON 78-79-5/RCT(L) 1191-16-8/PRO
D SCAN
E ESTER/CT
E ESTERS/CT

L12 23 SEA ABB=ON PLU=ON 64-19-7/RCT(L) (123-35-3/RCT OR
78-79-5/RCT)
D SCAN

L13 STR 123-35-3

L14 36 SEA SSS SAM L13 (448 REACTIONS)

L15 789 SEA SSS FUL L13 (11229 REACTIONS)
SAV L15 LAO307CRCT/A
E ESTERS/CT

L16 7147 SEA ABB=ON PLU=ON ESTERS+PFT, OLD, NT/CT

L17 7 SEA ABB=ON PLU=ON L15 AND L16
D SCAN
D SCAN
D QUE

SAV L17 LAO307CRCTA/A
L18 STR L13
L19 6 SEA SUB=L15 SSS SAM L18 (28 REACTIONS)
D SCAN
L20 88 SEA SUB=L15 SSS FUL L18 (708 REACTIONS)
SAV L20 LAO307CRCTB/A
L21 STR L18
L22 1 SEA SUB=L15 SSS SAM L21 (7 REACTIONS)
D SCAN
L23 5 SEA SUB=L15 SSS FUL L21 (16 REACTIONS)
D SCAN
SAV L23 LAO307CRCTC/A
L24 STR L21
L25 1 SEA SUB=L15 SSS SAM L24 (7 REACTIONS)
D SCAN
L26 7 SEA SUB=L15 SSS FUL L24 (38 REACTIONS)
D SCAN
SAV L26 LAO307CRCTD/A
SAV L27 LAO307CRCTE/A
L27 34 SEA ABB=ON PLU=ON (L10 OR L11 OR L12) OR L17 OR L23
OR L26
L28 43 SEA ABB=ON PLU=ON BABLER JAMES?/AU
L29 3 SEA ABB=ON PLU=ON L27 AND L28
SAV L29 LAO307CRCTIN/A
L30 31 SEA ABB=ON PLU=ON L27 NOT L29

FILE 'HCAPLUS' ENTERED AT 12:06:06 ON 16 MAY 2007

L31 QUE ABB=ON PLU=ON PY<2004 OR PRY<2004 OR AY<2004 OR
MY<2004 OR REVIEW/DT
L32 1 SEA ABB=ON PLU=ON L1 AND L31
D SCAN

FILE 'CASREACT' ENTERED AT 12:07:53 ON 16 MAY 2007

L33 25 SEA ABB=ON PLU=ON L30 AND L31
L34 3 SEA ABB=ON PLU=ON L29 AND L31

FILE 'HCAPLUS' ENTERED AT 12:08:48 ON 16 MAY 2007

D SCAN L1
L35 619 SEA ABB=ON PLU=ON L4/RACT
L36 5537 SEA ABB=ON PLU=ON L5/RACT
L37 86 SEA ABB=ON PLU=ON L6/P
L38 347 SEA ABB=ON PLU=ON L7/P
D 1-2 KWIC
L39 144 SEA ABB=ON PLU=ON L8/P
D KWIC
D 1-2 L36 KWIC
L40 0 SEA ABB=ON PLU=ON L36(L) L37
L41 12 SEA ABB=ON PLU=ON L36 AND L37
L42 0 SEA ABB=ON PLU=ON L35(L) (L38 OR L39)
L43 10 SEA ABB=ON PLU=ON L35 AND (L38 OR L39)
L44 20 SEA ABB=ON PLU=ON (L40 OR L41 OR L42 OR L43)
L45 34845 SEA ABB=ON PLU=ON L9
L46 70 SEA ABB=ON PLU=ON (L35 OR L36) AND L45
L47 4036 SEA ABB=ON PLU=ON L9/RACT
L48 50 SEA ABB=ON PLU=ON (L35 OR L36) AND L47
L49 9 SEA ABB=ON PLU=ON L48 AND L44
E ESTERS/CT
L50 QUE ABB=ON PLU=ON ESTERS+PFT,OLD,NT1/CT
L51 70 SEA ABB=ON PLU=ON L44 OR L46 OR (L48 OR L49)
L52 47 SEA ABB=ON PLU=ON L51 AND L50
E VITAMINS/CT
L53 QUE ABB=ON PLU=ON VITAMINS+PFT,OLD,NT/CT
E FLAVOR/CT
E FLAVORS/CT
E FLAVORING/CT
L54 QUE ABB=ON PLU=ON FLAVOR+PFT,OLD,NT/CT

L55 3 SEA ABB=ON PLU=ON L51 AND (L53 OR L54)
 D SCAN
 D SCAN L1
 E "DIETARY SUPPLEMENTS"/CT
 L56 QUE ABB=ON PLU=ON "DIETARY SUPPLEMENTS"+PFT,OLD,NT/CT
 L57 QUE ABB=ON PLU=ON "FLAVORING MATERIALS"+PFT,OLD,NT/CT
 L58 QUE ABB=ON PLU=ON "ODOR AND ODOROUS SUBSTANCES"+PFT,O
 LD,NT/CT
 L59 45 SEA ABB=ON PLU=ON L52 AND L31
 SAV L59 LAO307HCP/A
 L60 43 SEA ABB=ON PLU=ON L28
 D QUE
 L61 43 SEA ABB=ON PLU=ON L60 AND L31
 L62 QUE ABB=ON PLU=ON VITAM? OR ODOR? OR SMELL? OR
 PERFUM? OR SUPPLEMENT? OR FLAVOR?
 L63 4 SEA ABB=ON PLU=ON L61 AND L62
 L64 4 SEA ABB=ON PLU=ON L61 AND (L53 OR L56 OR L57 OR L58)
 D QUE
 L65 5 SEA ABB=ON PLU=ON L51 AND (L53 OR L56 OR L57 OR L58)
 L66 45 SEA ABB=ON PLU=ON L55 OR L59 OR L65
 L67 45 SEA ABB=ON PLU=ON L66 AND L31
 SAV L67 LAO307HCP/A
 L68 6 SEA ABB=ON PLU=ON L63 OR L64
 L69 13 SEA ABB=ON PLU=ON L61 AND L50
 L70 17 SEA ABB=ON PLU=ON L68 OR L69
 SAV L70 LAO307HCPIN/A
 D QUE L67
 L71 43 SEA ABB=ON PLU=ON L67 NOT L70
 D QUE L34
 D QUE L33

FILE 'CASREACT' ENTERED AT 12:45:36 ON 16 MAY 2007
 D QUE L33

FILE 'STNGUIDE' ENTERED AT 12:46:03 ON 16 MAY 2007

FILE 'MEDLINE, BIOSIS, DRUGU, EMBASE' ENTERED AT 12:46:36 ON 16 MAY 2007

L72 4 SEA ABB=ON PLU=ON L28
 D 1-4 TI
 SAV L72 LAO307IN/A

FILE 'STNGUIDE' ENTERED AT 12:47:53 ON 16 MAY 2007
 D QUE L34
 D QUE L70
 D QUE L72

FILE 'CASREACT, HCAPLUS, BIOSIS' ENTERED AT 12:49:46 ON 16 MAY 2007

L73 19 DUP REM L34 L70 L72 (5 DUPLICATES REMOVED)
 ANSWERS '1-3' FROM FILE CASREACT
 ANSWERS '4-18' FROM FILE HCAPLUS
 ANSWER '19' FROM FILE BIOSIS

FILE 'CASREACT' ENTERED AT 12:51:20 ON 16 MAY 2007

FILE 'CASREACT, HCAPLUS, BIOSIS' ENTERED AT 12:57:01 ON 16 MAY 2007

D L73 1-19 IBIB ABS

FILE 'CASREACT' ENTERED AT 12:57:02 ON 16 MAY 2007

FILE 'REGISTRY' ENTERED AT 12:57:42 ON 16 MAY 2007

D L4 IDE
D L5 IDE
D L6 IDE
D L7 IDE
D L8 IDE

FILE 'STNGUIDE' ENTERED AT 12:59:34 ON 16 MAY 2007

D QUE STAT L33
D QUE STAT L71

FILE 'CASREACT, HCAPLUS' ENTERED AT 13:00:44 ON 16 MAY 2007

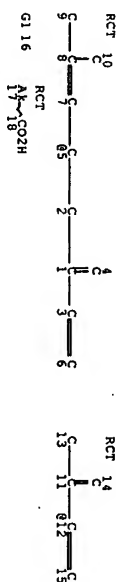
L74 67 DUP REM L33 L71 (1 DUPLICATE REMOVED)
ANSWERS '1-25' FROM FILE CASREACT
ANSWERS '26-67' FROM FILE HCAPLUS
D L74 1-25 IBIB ABS FHIT
D L74 26-67 IBIB ED ABS HITSTR HITIND

=> d his 134

L34 (FILE 'CASREACT' ENTERED AT 12:07:53 ON 16 MAY 2007)
 3 S L29 AND L31

=> d que 134

L10 1 SEA FILE-CASREACT ABB-ON PUU-ON 123-35-3/RCT(L) (105-8
 7-3/PRO OR 141-12-8/PRO)
 L11 2 SEA FILE-CASREACT ABB-ON PUU-ON 78-79-5/RCT(L) (1191-16
 -8/PRO)
 L12 23 SEA FILE-CASREACT ABB-ON PUU-ON 64-19-7/RCT(L) (123-35
 -3/RCT OR 78-79-5/RCT)
 L13 STR

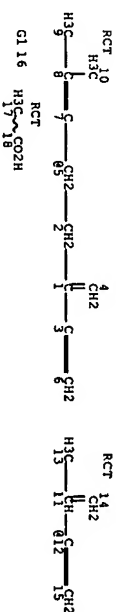


VAR G1=5/12
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ELEVEL IS LIMITED
 ECOUNT IS M1-X7 C AT 17

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

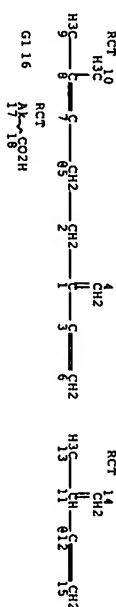
L15 789 SEA FILE-CASREACT SSS FUL L13 (11229 REACTIONS)
 L16 7147 SEA FILE-CASREACT ABB-ON PUU-ON ESTERS+PFT, OLD, NT/CT
 L17 7 SEA FILE-CASREACT ABB-ON PUU-ON L15 AND L16
 L21 STR



VAR G1=5/12
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 MLEVEL IS CLASS AT 2 4 5 6 9 10 11 13 14 15 17
 DEFAULT ELEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 18
 STEREO ATTRIBUTES: NONE

=> d que 170



VAR G1=5/12
 NODE ATTRIBUTES:
 CONNECT IS EI RC AT 17
 DEFAULT MLEVEL IS ATOM
 MLEVEL IS CLASS AT 2 4 5 6 9 10 11 13 14 15
 DEFAULT ELEVEL IS LIMITED
 ECOUNT IS M1-X7 C AT 17

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L26 7 SEA FILE-CASREACT SUB-L15 SSS FUL L24 (38 REACTIONS
)
 L27 34 SEA FILE-CASREACT ABB-ON PUU-ON (L10 OR L11 OR L12)
 OR L17 OR L21 OR L26
 L28 43 SEA FILE-CASREACT ABB-ON PUU-ON BABLER JAMES7/AN
 L29 3 SEA FILE-CASREACT ABB-ON PUU-ON L27 AND L28
 L31 QUE ABB-ON PUU-ON P1<2004 OR P1<2004 OR AY<2004 OR
 M1<2004 OR REVIEW/DI
 L34 3 SEA FILE-CASREACT ABB-ON PUU-ON L29 AND L31

=> d his 170

(FILE 'HCAPIUS' ENTERED AT 12:08:48 ON 16 MAY 2007)
 L70 17 S L68 OR L69

L28 43 SEA FILE-CASREACT ABB-ON PUU-ON BABLER JAMES7/AN
 L31 QUE ABB-ON PUU-ON P1<2004 OR P1<2004 OR AY<2004 OR
 M1<2004 OR REVIEW/DI
 L50 QUE ABB-ON PUU-ON ESTERS+PFT, OLD, NT/CT
 L53 QUE ABB-ON PUU-ON VITAMINS+PFT, OLD, NT/CT
 L56 QUE ABB-ON PUU-ON DIETARY SUPPLEMENTS+PFT, OLD, NT/C
 L57 QUE ABB-ON PUU-ON *FLAVORING MATERIALS+PFT, OLD, NT/C
 L58 QUE ABB-ON PUU-ON *ODOR AND ODOROUS SUBSTANCES+PFT,
 OLD, NT/CT
 L60 43 SEA FILE-HCAPIUS ABB-ON PUU-ON L28
 L61 43 SEA FILE-HCAPIUS ABB-ON PUU-ON L60 AND L31
 L62 QUE ABB-ON PUU-ON VITAM? OR ODO? OR SHEL? OR PERU
 NT OR SUPPLEMENT? OR FLAVOR?
 L63 4 SEA FILE-HCAPIUS ABB-ON PUU-ON L61 AND L62
 L64 4 SEA FILE-HCAPIUS ABB-ON PUU-ON L61 AND L56
 L65 OR L57 OR L58)
 L66 6 SEA FILE-HCAPIUS ABB-ON PUU-ON L63 OR L64
 L68 13 SEA FILE-HCAPIUS ABB-ON PUU-ON L61 AND L50
 L70 17 SEA FILE-HCAPIUS ABB-ON PUU-ON L68 OR L69

=> d his 172
(FILE 'MEDLINE, BIOSIS, DRUGU, EMBASE' ENTERED AT 12:46:36 ON 16 MAY 2007)
L72 4 S L28
SAV L72 LA0307IN/A

FILE 'STINGUIDE' ENTERED AT 12:47:53 ON 16 MAY 2007

=> d que 172
L72 43 SEA FILE-CASREACT ABB-ON PLU-ON BABLER JAMES7/AU
L72 4 SEA L28

=> dup rem 134 170 172
FILE 'CASREACT' ENTERED AT 12:49:46 ON 16 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'HCAPLUS' ENTERED AT 12:49:46 ON 16 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE 'BIOSIS' ENTERED AT 12:49:46 ON 16 MAY 2007
COPYRIGHT (C) 2007 The Thomson Corporation
PROCESSING COMPLETED FOR L34
PROCESSING COMPLETED FOR L70
PROCESSING COMPLETED FOR L72
19 DUP REM 134 170 172 (5 DUPLICATES REMOVED)

ANSWERS '1-3' FROM FILE CASREACT
ANSWERS '4-18' FROM FILE HCAPLUS
ANSWER '19' FROM FILE BIOSIS

INVENTOR SEARCH RESULTS

=> d l73 1-19 1bib abs
YOU HAVE REQUESTED DATA FROM FILE 'CASREACT, HCAPLUS, BIOSIS' - CONTINUE
? (Y)/N:Y

L73 ANSWER 1 OF 19 CASREACT COPYRIGHT 2007 ACS ON STN DUPLICATE 1
ACCESSION NUMBER: 142:463897 CASREACT Full-text
TITLE: Processes for synthesizing esters by
1,4-addition of alkanolic acids to myrcene or
isoprene

INVENTOR(S): Babler, James H.
PATENT ASSIGNEE(S): Loyola University of Chicago, USA
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXDZ
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
MO 2005044774	A1	20050519	MO 2004-0522075	20040708
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, GU, HT, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, ME, MK, MN, MW, MX, MY, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SN, SY, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MM, MZ, NA, SD, SI, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2007055076	A1	20070308	US 2006-564307	20061017
			US 2003-486781P	20030711
			MO 2004-0522075	20040708

PRIORITY APPLN. INFO.:
OTHER SOURCE(S): MARPAT 142:463897
AB A process was disclosed for synthesizing esters RCO2R1 (R = allyl; R1 = monoterpene moiety) which can be used in the manufacture of citral, precursors to citral and other products, such as vitamins, nutritional supplements, flavorings and fragrances. The process includes a 1,4-addition of an alkanolic acid to the conjugated diene of myrcene, which can be generated from β -pinene, or the conjugated diene of isoprene to produce esters thereof. Thus, myrcene was refluxed with AcONa/AcOH in Clph for 20 h to form a 70:30 mixture of geranyl acetate and neryl acetate in 60% yield.
REFERENCE COUNT: 4
THERE ARE 4 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L73 ANSWER 2 OF 19 CASREACT COPYRIGHT 2007 ACS ON STN DUPLICATE 2
ACCESSION NUMBER: 135:16653 CASREACT Full-text
TITLE: Methods for conversion of isoprene to prenyl alcohol and esters
INVENTOR(S): Babler, James H.
PATENT ASSIGNEE(S): Loyola University of Chicago, USA
SOURCE: U.S., 7 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO. 6278016
 KIND B1
 DATE 20010821
 APPLICATION NO. US 1999-458153
 DATE 19991209
 PRIORITY APPL. INFO. US 1999-458153
 OTHER SOURCE(S): MARPAT 135:16653
 AB Methods for preparing ester derivs. of 3-methyl-2-buten-1-ol (prenyl alc.) from the addition reaction of isoprene with alkenoic acids (e.g., acetic acid-acetic anhydride mixture) in the presence of an inorg. acid (e.g., phosphoric acid) catalyst are disclosed. The resultant prenyl ester (e.g., prenyl acetate) readily can be converted to prenyl alc. by saponification
 REFERENCE COUNT: 26
 THERE ARE 26 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L73 ANSWER 3 OF 19 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 84:150125 CASREACT Full-text
 TITLE: A facile route to E-4-bromo-3-methyl-2-buten-1-ol. Application to the stereoselective synthesis of trisubstituted olefins
 AUTHOR(S): Babler, James H.; Butner, William J.
 CORPORATE SOURCE: Dep. Chem., Loyola Univ., Chicago, Chicago, IL, USA
 SOURCE: Tetrahedron Letters (1976), (4), 239-42
 CODEN: TETL; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Addition of N-bromosuccinimide to isoprene in AcOH at 25° gave, after fractional distillation, 58% AcOCH₂CH=CMeCH₂Br, which on hydrolysis and treatment with NaH gave (E)-ROCH₂CH=CMeCH₂Br (1, R = H). Reaction of 1, (R = H, Ac) with Bu₂CuLi gave HOCH₂CH=CMeCH₂Br and BuCH₂CH=CMeCH₂Br, resp.

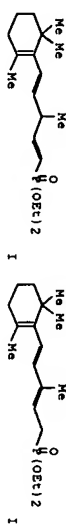
L73 ANSWER 4 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 3
 ACCESSION NUMBER: 2000:238081 HCAPLUS Full-text
 DOCUMENT NUMBER: 132:264887
 TITLE: Method of preparing 3-(3-methyl-2-buten-1-yl)-2,4-pentanedione and related dicarbonyl compounds
 INVENTOR(S): Babler, James H.; Posvic, Harvey W.
 PATENT ASSIGNEE(S): Loyola University of Chicago, USA
 SOURCE: U.S., 9 PP.
 DOCUMENT TYPE: Patent
 CODEN: USXXAM
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION: Patent

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6049010	A	20000411	US 1998-161983	1998 0929
			US 1998-161983	1998 0929

PRIORITY APPL. INFO.:
 OTHER SOURCE(S): CASREACT 132:264887; MARPAT 132:264887
 AB A method for preparation of a dicarbonyl compound by reacting a conjugated alkadiene compound with a 1,3-dicarbonyl compound in the presence of an acid catalyst is

described. E.g., polyphosphoric acid catalyzed the reaction of 2,4-pentanedione with isoprene to give 59% 3-(3-methyl-2-buten-1-yl)-2,4-pentanedione.
 REFERENCE COUNT: 35
 THERE ARE 35 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L73 ANSWER 5 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 4
 ACCESSION NUMBER: 1993:124810 HCAPLUS Full-text
 DOCUMENT NUMBER: 118:124810
 TITLE: An expedient route to a versatile intermediate for the stereoselective synthesis of all-trans-retinoic acid and beta-carotene
 AUTHOR(S): Babler, James H.; Schlidt, Scott A.
 CORPORATE SOURCE: Dep. Chem., Loyola Univ., Chicago, IL, 60626, USA
 SOURCE: Tetrahedron Letters (1992), 33(50), 7697-706
 CODEN: TETL; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 118:124810



AB Base-catalyzed isomerization of phosphonate I afforded the corresponding allylic phosphonate II as the sole product. Horner-Emmons olefination of Et trans-3-methyl-4-oxo-2-butenate with the ylide derived from II concludes a facile synthesis of the all-trans stereoisomer of Et retinoate.

L73 ANSWER 6 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1998:621182 HCAPLUS Full-text
 DOCUMENT NUMBER: 129:230459
 TITLE: Methods for preparing prenyl alcohol
 INVENTOR(S): Babler, James H.
 PATENT ASSIGNEE(S): Loyola University of Chicago, USA
 SOURCE: PCT Int. Appl., 28 PP.
 DOCUMENT TYPE: Patent
 CODEN: PIXX02
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION: Patent

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9840345	A1	19980917	WO 1998-US256	1998 0108

W: AU, BR, CA, CN, ID, IL, JP, KP, KR, MX, AM, AZ, BY, KG,
 KZ, MD, RU, TJ, TM
 RA: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC,
 NL, PT, SE
 A 19990216 US 1997-814472
 US 5872277

CA 2281756 A1 19980917 CA 1998-2281756 <--
 1998
 0108
 AU 9658171 A 19980929 AU 1998-58171 <--
 1998
 0108
 EP 968170 A1 20000105 EP 1998-901716 <--
 1998
 0108
 R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE
 JP 2001514652 T 20010911 JP 1998-539550 <--

PRIORITY APPL. INFO.:
 US 1997-814472 A <--
 1997
 0310
 WO 1998-US256 W <--
 1998
 0108

OTHER SOURCE(S): CASREACT 129:230459; MARPAT 129:230459
 AB Methods for preparing 3-methyl-2-buten-1-ol (prenyl alc.) from 2-methyl-1,3-butadiene (isoprene) and carboxylic acids are disclosed. Carboxylic acids which can be used in the process have a K_{ow} relative to water greater than 10-4; dichloroacetic acid is especially preferred. The process involves the slow (e.g., dropwise) addition of isoprene to the carboxylic acid to form a prenyl ester. The ester-formation reaction proceeds at room temperature in most cases; use of an organic base catalyst, preferably a sodium or potassium salt of the reactant carboxylic acid, improves the yield. The resultant prenyl ester can be converted to prenyl alc. by reaction with a base. Prenyl alc. can be readily converted to citral, a chemical intermediate in the synthesis of vitamins A and E, and several widely-used carotenoids. Thus, isoprene was treated with dichloroacetic acid and sodium dichloroacetate at room temperature (with addns. of isoprene during the course of the reaction) to give 71% 3-methyl-2-butenyl dichloroacetate. This ester was further saponified to give 88% the expected 3-methyl-2-butenyl alc. Carrying out this experiment without the sodium dichloroacetate gave a product mixture containing only <50% the desired ester.
 REFERENCE COUNT: 4
 THERE ARE 4 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L73 ANSWER 7 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1996:1242785 HCAPLUS Full-text
 DOCUMENT NUMBER: 124:343745
 TITLE: A facile route to 3-alkoxy-3-methylpropenals, useful intermediates in the synthesis of carotenoids
 AUTHOR(S): Babelier, James H.; Lipcak, Vincent F.; Treutmann, Jeffrey A.; Zayia, Gregory H.
 CORPORATE SOURCE: Dep. Chemistry, Loyola Univ., Chicago, Chicago, IL, 60626, USA
 SOURCE: Synthetic Communications (1996), 26(10), 1943-51
 CODEN: SYNCAV; ISSN: 0039-7911
 PUBLISHER: Dekker
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 124:343745
 AB A "one-pot" process for the preparation of a carotenoid synthon, EtOCH:CH=CHCHO, has been developed that involves methoxide-promoted condensation of propionaldehyde with Me

L73 ANSWER 8 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1996:13322 HCAPLUS Full-text
 DOCUMENT NUMBER: 124:176588
 TITLE: Method of making 2,7-dimethyl-2,4,6-octatrienol, a key intermediate in the commercial syntheses of various carotenoids
 INVENTOR(S): Babelier, James H.
 PATENT ASSIGNEE(S): Loyola University of Chicago, USA
 SOURCE: U.S., 9 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

 US 5471005 A 19951128 US 1994-339659 1994
 1118

WO 9616013 A1 19960530 WO 1995-US13372 <--
 1995
 1011
 W: AU, CA, JP, KP, KR
 RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
 AU 9639601 A 19960617 AU 1995-39601 <--
 1995
 1011

PRIORITY APPL. INFO.:
 US 1994-339659 A <--
 1994
 1118
 WO 1995-US13372 W <--
 1995
 1011

OTHER SOURCE(S): CASREACT 124:176588
 AB A procedure for forming methylmalonaldehyde from propionaldehyde, an alkyl formate and a sodium alkoxide, utilizing a crossed-Claisen condensation is disclosed. The procedure avoids the formation of aldol condensation products. Also disclosed are processes for preparing 3-alkoxy-2-methylpropenals such as 2-methyl-3-(2-methyl-2-propenoxy)propenal from methylmalonaldehyde. The latter products are useful in the synthesis of carotenoids.

L73 ANSWER 9 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1994:57133 HCAPLUS Full-text
 DOCUMENT NUMBER: 121:157133
 TITLE: Process for preparing 6,10,14-trimethyl-4-pentadecyn-6-ols
 INVENTOR(S): Babelier, James H.
 PATENT ASSIGNEE(S): Loyola University of Chicago, USA
 SOURCE: PCT Int. Appl., 57 pp.
 CODEN: PFXMDZ
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 16

SN 10/564307 Page 9 of 139 STIC STN SEARCH 5/17/2007

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
MO 9412457	A1	19940609	MO 1993-US10276	1993 1027
W: AU, CA, JP, KR, PT, SE RM: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL,				
JP 2002072251	A	20020312	JP 2001-160650	1991 0216
JP 2002100781	A	20020405	JP 2001-160671	1991 0216
JP 2003222838	A	20030808	JP 2002-331795	1991 0216
JP 3447730	B2	20030916		
JP 2000292813	A	20001020	JP 2000-2212	1991 0327
JP 2000330139	A	20001130	JP 2000-121941	1991 0327
JP 2001186257	A	20010710	JP 2000-342919	1991 0327
JP 10213819	A	19980811	JP 1998-38120	1991 0511
JP 11233791	A	19980827	JP 1998-323157	1991 0511
JP 2001144304	A	20010525	JP 2000-304158	1991 0511
JP 2000004024	A	20000107	JP 1999-153145	1992 0121
JP 3501977	B2	20040302		
JP 2000031498	A	20000128	JP 1999-187097	1992 0121
JP 09165791	A	19970624	JP 1996-294546	1992 0124
JP 05072564	A	19930326	JP 1992-59403	1992 0213

Page 9

SN 10/564307 Page 10 of 139 STIC STN SEARCH 5/17/2007

US 5218464

A

19930608

US 1992-836797

1992 0218

US 5349071	A	19940920	US 1992-976219	1992 1125
AU 9456644	A	19940622	AU 1994-56644	1993 1027
CN 1092758	A	19940928	CN 1993-120597	1993 1124
US 5410094	A	19950425	US 1994-255369	1994 0608
JP 08298331	A	19961112	JP 1996-85713	1996 0417
JP 2652366	B2	19970910		
JP 10041520	A	19980213	JP 1997-102689	1997 0404
JP 2890037	B2	19990510		
JP 10223910	A	19980821	JP 1998-38121	1998 0204
JP 3057049	B2	20000626		
JP 2002033332	A	20020131	JP 2001-142474	2001 0511
JP 3380546	B2	20030224		
JP 2004004890	A	20040108	JP 2003-168989	2003 0613
JP 3554563	B2	20040818		
JP 2004006550	A	20040108	JP 2003-271415	2003 0707
JP 2004258681	A	20040916	JP 2004-150976	2004 0520
JP 2004310123	A	20041104	JP 2004-150975	2004 0520
JP 2004334224	A	20041125	JP 2004-150974	2004 0520
PRIORITY APPLN. INFO.:				
			US 1992-976219	A
			JP 1991-77318	A1

Page 10

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<--	JP 2000-13650	A3	0216
<--	JP 1997-215955	A3	0216
<--	JP 2000-2212	A3	0327
<--	JP 2000-342919	A3	0327
<--	JP 1995-335554	A3	0511
<--	JP 1998-38120	A3	0511
<--	JP 1998-38121	A3	0511
<--	JP 1998-124729	A3	0121
<--	JP 1999-153145	A3	0121
<--	JP 1992-34194	A3	0124
<--	JP 1992-38637	A3	0129
<--	JP 1992-187604	A3	0622
<--	MO 1993-US10276	W	1027
<--	JP 2001-92845	A3	0328

CASREACT 121:157133; MARPAT 121:157133
AB Tertiary alkynols Me2CH(CH2)3C(OH)MeC(Cp)bond,CCCH2CH(OR)Me (R = H, alkyl, alkenyl, alkoxyalkyl, trialkylsilyl, arylalkyl) (e.g., 1-(1-octynyl)cyclohexanol).

L73 ANSWER 10 OF 19	HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:	1991:649580 HCAPLUS Full-text
DOCUMENT NUMBER:	119:249580
TITLE:	Method of preparing C-18 ketones used in the preparation of vitamins E and K
INVENTOR(S):	Babier, James H.
PATENT ASSIGNEE(S):	Loyola University of Chicago, USA
SOURCE:	U.S., 13 pp.
DOCUMENT TYPE:	CODEN: USXXAM
LANGUAGE:	Patent
FAMILY ACC. NUM. COUNT:	English
PATENT INFORMATION:	1
PATENT NO.	KIND DATE APPLICATION NO. DATE
US 5231232	A 19930727 US 1991-807462
PRIORITY APPL. INFO.:	<--
US 1991-807462	1991 1218

OTHER SOURCE(S): CASREACT 119:249580
AB Methods for preparing unsatd. C-18 ketones which can be used in the synthesis of vitamins E and K are claimed. One procedure involves coupling a C-9 primary allylic halide to a carbonyl-group-containing C-9 terminal alkyne. A second, two-step procedure employs a C-4 bisallylic halide (molar excess) and a carbonyl-group-containing C-9 terminal alkyne to form a C-13 primary allylic halide. The C-13 primary allylic halide can then be converted to the desired C-18 ketone by reaction with 2-methyl-3-buten-2-ol. Novel C-18 ketones (e.g., 14-hydroxy-6,14-dimethyl-10-methylene-5-pentadecene-7,12-diyne-2-one), C-13 allylic halides (e.g., 10-chloromethyl-6-methyl-5,10-undecadiene-7-yn-2-one) and C-9 allylic halides (e.g., 6-chloromethyl-2-methyl-6-hepten-3-yn-2-ol) are formed in the process.

L73 ANSWER 11 OF 19	HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:	1992:490545 HCAPLUS Full-text
DOCUMENT NUMBER:	117:90545
TITLE:	Method of making 2,7-dimethyl-2,4,6-octatrienediol and derivatives thereof
INVENTOR(S):	Babier, James H.
PATENT ASSIGNEE(S):	Loyola University of Chicago, USA
SOURCE:	U.S., 9 pp.
DOCUMENT TYPE:	CODEN: USXXAM
LANGUAGE:	Patent
FAMILY ACC. NUM. COUNT:	English
PATENT INFORMATION:	1
PATENT NO.	KIND DATE APPLICATION NO. DATE
US 5107030	A 19920421 US 1991-661722
US 9215544	A1 19920917 MO 1992-US1462
	1992 0304

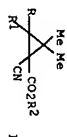
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4567265	A	19860128	US 1984-570874	1984 0116

PRIORITY APPL. INFO.:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 1984-570874				1984 0116

OTHER SOURCE(S): CASREACT 105:43114; MARPAT 105:43114
GI



AB The title compds. (I; R = H, R1 = (halo)alkyl, (halo)alkenyl, cycloalkyl, cycloalkenyl, alkoxyacetyl, naphthyl, furyl, thieryl, pyridinyl, pyrrolyl, indolyl, (un)substituted Ph; R1 = (CH2)n, CH2CH2CH2CH2; R2 = Me, Et; Z = O, S, Mev; n = 3-5), intermediates for pyrethroids, were prepared by cycloaddn. of R1C(CN)CO2R2 with Me2CHNO2 in alc. solvents in presence of a base. Thus, NCCH2CO2Et and BzH were refluxed in HOAc containing β-alanine to give 92% (E)-PhCH=C(CN)CO2Et which was refluxed with Me2CHNO2 in EtOH containing NaOEt to give 96% I (R = H, R1 = Ph, Ph and CN cis).

L73 ANSWER 16 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:203561 HCAPLUS Full-text
DOCUMENT NUMBER: 102:203561
TITLE: A facile method for the conversion of primary alkyl chlorides to the corresponding bromides
AUTHOR(S): Babler, James H.; Spina, Kenneth P.
CORPORATE SOURCE: Dep. Chem., Loyola Univ., Chicago, IL, 60626, USA
SOURCE: Synthetic Communications (1984), 14(14), 1313-19
CODEN: SYNCAV; ISSN: 0039-7911

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:203561
AB The exchange reaction of RCH2Cl (R = 1-pentadecyl, MeCOCH2CH2CH2, 2-ClC6H4, CH2CH2CO2Et) with NaBr gave the resp. RCH2Br. 1-Chlorononadecane was refluxed with NaBr, DMF, and CH2Br2 at 100° to give 1-bromononadecane. Similarly, (ClCH2CH2)2O was converted to (BrCH2CH2)2O.

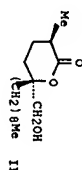
L73 ANSWER 17 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:586089 HCAPLUS Full-text
DOCUMENT NUMBER: 93:186089
TITLE: Lactone formation via oxidative cyclization of an unsaturated carboxylic acid: application to the stereoselective synthesis of (+)-malynolide, an antibiotic from the marine blue-green alga *Lyngbya majuscula* Gomont

AUTHOR(S): Gomont, James H.; Invergo, Benedict J.; Sarnesi, Steven J.

CORPORATE SOURCE:

SOURCE: Dep. Chem., Loyola Univ., Chicago, IL, 60626, USA

DOCUMENT TYPE: Journal of Organic Chemistry (1980), 45(21), 4241-3
LANGUAGE: English
OTHER SOURCE(S): CODEN: JOCEAH; ISSN: 0022-3263
CASREACT 93:186089



AB Treatment of Me(CH2)8C(CH2)2CHMeCO2H (I) with 3-ClC6H4CO3H, followed by heating the intermediate epoxide in refluxing cyclohexane, afforded (+)-malynolide (II), a recently isolated marine natural product, in 50% yield. The olefinic acid I was in turn prepared in 5 steps from Me(CH2)8CHO, the key step involving a Michael reaction between MeCH(CO2Et)2 and 1-dodecen-3-one.

L73 ANSWER 18 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:449207 HCAPLUS Full-text
DOCUMENT NUMBER: 81:49207
TITLE: Facile method for the bismethylation of ketones to functionalized trisubstituted olefins
AUTHOR(S): Babler, James H.; Olsen, Douglas O.
CORPORATE SOURCE: Dep. Chem., Loyola Univ., Chicago, IL, USA
SOURCE: Tetrahedron Letters (1974), (4), 351-4
CODEN: TELEAV; ISSN: 0040-4039

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 81:49207
AB R1C(OH)CH : CH2, prepared from R1CO(R = R1 = Ph; R, R1 = (CH2)5; R = Me, R1 = Ph, (CH2)4Me, CH : CH2], with AcOH-Ac2O gave 55-91% R1C : CHCH2OAc.

L73 ANSWER 19 OF 19 BIOSIS COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 1993:417023 BIOSIS Full-text
DOCUMENT NUMBER: PREV19934506468
TITLE: A facile route to allylic phosphonates via base-catalyzed isomerization of the corresponding vinyl phosphonates.
AUTHOR(S): Kiddle, James V.; Babler, James H. [Reprint author]

CORPORATE SOURCE: Dep. Chem., Loyola Univ., Chicago, Chicago, IL 60626, USA
SOURCE: Journal of Organic Chemistry, (1993) Vol. 58, No. 13, pp. 3572-3574.
CODEN: JOCEAH; ISSN: 0022-3263.

DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 15 Sep 1993
Last Updated on STN: 6 Nov 1993

SN 10/564307 Page 17 of 139 STIC STN SEARCH 5/17/2007
 REGISTRY MOLECULES OF INTEREST

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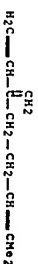
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14 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS ON STN
 RN 123-35-3 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 1,6-octadiene, 7-methyl-3-methylene- (CA INDEX NAME)
 OTHER NAMES:

CN β -geraniolene
 CN β -myrcene
 CN 2-methyl-6-methylene-2,7-octadiene
 CN 3-methylene-7-methyl-1,6-octadiene
 CN 7-methyl-3-methylene-1,6-octadiene
 CN Myrcene
 CN NSC 406264
 DR 2153-31-3
 MF C10 H16
 CI COM

STN files: AGRICOLA, ANABSTR, BELISTEIN, BIOSIS, BIOTECNO, CA, CAB, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DETHERM, DRUGO, EMBASE, GHELIN, HSDB, IFCDB, IFIPAT, IFIUD, IPA, MEDLINE, MRCK, MSDS-OHS, NARALERT, PIRA, PROMT, RTECS, SPECINFO, SYNTLINE, TOXCENTER, ULIDAT, USPAT2, USPATFULL

(*File contains numerically searchable property data)
 Other Sources: DSL, EINECS, TSCA
 (**Enter CHEMLIST file for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10169 REFERENCES IN FILE CA (1907 TO DATE)
 51 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 10250 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 89 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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 1 S 78-79-5/RN

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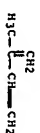
15 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS ON STN
 RN 78-79-5 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 1,3-butadiene, 2-methyl- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Isoprene (8C1)
 OTHER NAMES:
 CN β -methylbutvinyl

SN 10/564307 Page 18 of 139 STIC STN SEARCH 5/17/2007

CN 2-methyl-1,3-butadiene
 CN 2-methylbutadiene
 CN 3-methyl-1,3-butadiene
 CN Isoprene
 CN NSC 9237
 DR 823271-95-0, 78006-92-5
 MF C5 H8
 CI COM

STN files: AGRICOLA, ANABSTR, AQUIRE, BELISTEIN, BIOSIS, BIOTECNO, CA, CAOLD, CAPLUS, CASREACT, CSNB, CHEMCATS, CHEMINFORMX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, GHELIN, HSDB, IFCDB, IFIPAT, IFIUD, IPA, MEDLINE, MRCK, MSDS-OHS, NARALERT, PIRA, PROMT, PS, RTECS, SPECINFO, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VTB

(*File contains numerically searchable property data)
 Other Sources: DSL, EINECS, TSCA
 (**Enter CHEMLIST file for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

12878 REFERENCES IN FILE CA (1907 TO DATE)
 596 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 12893 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 21 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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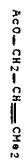
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16 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS ON STN
 RN 1191-16-8 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 2-Buten-1-ol, 3-methyl-, acetate (6CI, 7CI, 8CI, 9CI)
 OTHER NAMES:

CN 1,7-Dimethylallyl acetate
 CN 1-Acetoxy-3-methyl-2-butene
 CN 3,3-Dimethylallyl acetate
 CN 3-Methyl-1-acetoxy-2-butene
 CN 3-Methyl-2-buten-1-ol acetate
 CN 3-Methyl-2-buten-1-yl acetate
 CN 3-Methyl-2-butenyl acetate
 CN Acetic acid 3-methyl-2-butenyl ester
 CN Dimethylallyl acetate
 CN Isopent-2-enyl acetate
 CN Prenyl acetate
 MF C7 H12 O2
 CI COM

STN files: AGRICOLA, ANABSTR, BELISTEIN, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMX, CHEMLIST, CIN, CSCHEM, IFCDB, IFIPAT, IFIUD, RTECS, SPECINFO, TOXCENTER, USPAT2, USPATFULL

(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMIST file for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

333 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
333 REFERENCES IN FILE CAPLUS (1907 TO DATE)
8 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d his 17

L7 (FILE 'REGISTRY' ENTERED AT 10:25:28 ON 16 MAY 2007)
1 S 105-87-3/RN

=> d 17 ide

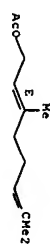
L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 105-87-3 REGISTRY
ED Entered STN: 16 Nov 1984
2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

OTHER CA INDEX NAMES:
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (2E)- (9CI)
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (E)- (8CI)
CN Geraniol acetate (6CI)

OTHER NAMES:
CN (E)-3,7-Dimethyl-2,6-octadien-1-ol acetate
CN (E)-3,7-Dimethyl-2,6-octadienyl acetate
CN β -Geranyl acetate
CN Acetic acid geraniol ester
CN Bay pine (oyster) oil
CN Geranyl acetate
CN Geranyl ethanoate
CN NSC 2364
CN trans-1-Acetoxy-3,7-dimethyl-2,6-octadiene
CN trans-3,7-Dimethyl-2,6-octadien-1-yl acetate
CN trans-Geranyl acetate
FS STEREOSEARCH
DR 8022-83-1, 130396-84-8
MF C12 H20 O2
CI COM

STN Files: AGRICOLA, ANABSTR, BELSTEIN, BIOSIS, BIOTECNO, CA, CAOLD, CAPLUS, CASREACT, CANB, CHEMCATS, CHEMINFORMRX, CHEMIST, CINC, CSCHEM, DDFU, DETHERM, DRUGU, EMASE, GHELIN, HSDB, IFCDB, IFIPAT, IFIUD, IPA, MSDS-ONS, NABALERT, PROMT, RTECS, SPECINFO, TOXCENTER, USPAT2, USPATFUL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMIST file for up-to-date regulatory information)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3624 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3648 REFERENCES IN FILE CAPLUS (1907 TO DATE)
63 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d his 18

L8 (FILE 'REGISTRY' ENTERED AT 10:25:28 ON 16 MAY 2007)
1 S 141-12-8/RN

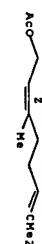
=> d 18 ide

L8 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 141-12-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

OTHER CA INDEX NAMES:
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (2Z)- (9CI)
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (Z)- (8CI)
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, formate, cis- (7CI)
CN Nerol acetate (6CI)

OTHER NAMES:
CN cis-1-Acetoxy-3,7-dimethyl-2,6-octadiene
CN cis-Geranyl acetate
CN Neryl acetate
CN STEREOSEARCH
DR 130396-85-9
MF C12 H20 O2
CI COM
SR CAS EARLY REGISTRATIONS
STN Files: AGRICOLA, ANABSTR, BELSTEIN, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMIST, CSCHEM, DDFU, DRUGU, GHELIN, IFCDB, IFIPAT, IFIUD, NABALERT, RTECS, SPECINFO, TOXCENTER, USPAT2, USPATFUL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMIST file for up-to-date regulatory information)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1605 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1616 REFERENCES IN FILE CAPLUS (1907 TO DATE)
27 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

STRUCTURE SEARCH

=> d his 133

(FILE 'HCAPIUS' ENTERED AT 12:06:06 ON 16 MAY 2007)

L13 FILE 'CASREACT' ENTERED AT 12:07:53 ON 16 MAY 2007
25 S L30 AND L31

=> d que stat 133

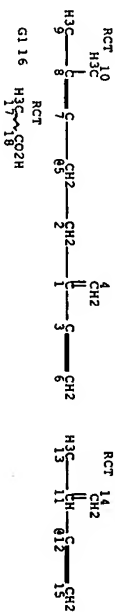
L10 1 SEA FILE-CASREACT ABB-ON PUU-ON 123-35-3/RCT(L) (105-8
7-3/PRO OR 141-12-8/PRO)
L11 2 SEA FILE-CASREACT ABB-ON PUU-ON 78-79-5/RCT(L) (1191-16
-8/PRO)
L12 23 SEA FILE-CASREACT ABB-ON PUU-ON 64-19-17/RCT(L) (123-35
-3/RCT OR 78-79-5/RCT)
L13 STR



VAR G1-5/12
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ELEVEL IS LIMITED
ECOUNT IS M1-X7 C AT 17
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L15 789 SEA FILE-CASREACT SSS FUL L13 (11229 REACTIONS)
L16 7147 SEA FILE-CASREACT ABB-ON PUU-ON ESTERS+PTT,OLD,NT/CT
L17 7 SEA FILE-CASREACT ABB-ON PUU-ON L15 AND L16
L21 STR

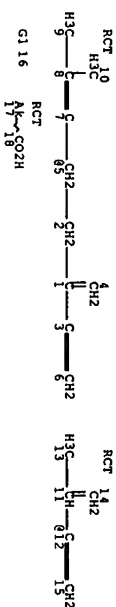


VAR G1-5/12
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ELEVEL IS LIMITED
ECOUNT IS M1-X7 C AT 17
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L23 5 SEA FILE-CASREACT SUB-L15 SSS FUL L21 (16 REACTIONS)

L24 STR



VAR G1-5/12
NODE ATTRIBUTES:
CONNECT IS EL RC AT 17
DEFAULT MLEVEL IS ATOM
DEFAULT ELEVEL IS LIMITED
ECOUNT IS M1-X7 C AT 17
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18

L26 7 SEA FILE-CASREACT SUB-L15 SSS FUL L24 (38 REACTIONS)
L27 34 SEA FILE-CASREACT ABB-ON PUU-ON (L10 OR L11 OR L12)
OR L17 OR L23 OR L26
L28 43 SEA FILE-CASREACT ABB-ON PUU-ON BABLER JAMEST/NU
L29 3 SEA FILE-CASREACT ABB-ON PUU-ON L27 AND L28
L30 31 SEA FILE-CASREACT ABB-ON PUU-ON L27 NOT L29
L31 QUE ABB-ON PUU-ON PY<2004 OR PRY<2004 OR AY<2004 OR
MY<2004 OR REVIEW/DT
L33 25 SEA FILE-CASREACT ABB-ON PUU-ON L30 AND L31

=> d his 171

(FILE 'HCAPIUS' ENTERED AT 12:08:48 ON 16 MAY 2007)

L71 43 S L67 NOT L70

=> d que stat 171
L2 35 SEA FILE-REGISTRY ABB-ON PUU-ON (100-66-3/BI OR
105-87-3/BI OR 105-90-8/BI OR 105-91-9/BI OR 106-24-1/B
I OR 106-25-2/BI OR 106-42-3/BI OR 107-92-6/BI OR
108-21-4/BI OR 108-88-3/BI OR 108-90-7/BI OR 108-94-1/B
I OR 109-20-6/BI OR 1191-16-8/BI OR 123-35-3/BI OR
123-66-4/BI OR 127-08-2/BI OR 127-09-3/BI OR 137-40-6/B
I OR 138-86-3/BI OR 141-12-8/BI OR 142-96-1/BI OR
157256-67-8/BI OR 19559-59-2/BI OR 3915-83-1/BI OR
503-74-2/BI OR 5392-40-5/BI OR 556-82-1/BI OR 64-19-7/B
I OR 78-79-5/BI OR 78-93-3/BI OR 79-09-4/BI OR
79-31-2/BI OR 80-26-2/BI OR 851785-97-2/BI)
L4 1 SEA FILE-REGISTRY ABB-ON PUU-ON 123-35-3/RN
L5 1 SEA FILE-REGISTRY ABB-ON PUU-ON 78-79-5/RN
L6 1 SEA FILE-REGISTRY ABB-ON PUU-ON 1191-16-8/RN
L7 1 SEA FILE-REGISTRY ABB-ON PUU-ON 105-87-3/RN
L8 1 SEA FILE-REGISTRY ABB-ON PUU-ON 141-12-8/RN
L9 11 SEA FILE-REGISTRY ABB-ON PUU-ON L2 AND FACETATE7/CNS

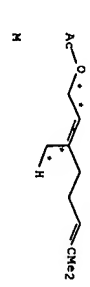
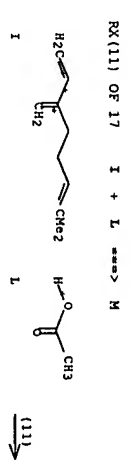
128 43 SEA FILE-CASREACT ABB-ON PLU-ON BABLER JAMES7/NU
 129 QUE ABB-ON PLU-ON PY<2004 OR PRY<2004 OR AY<2004 OR
 130 MY<2004 OR REVIEW/DT
 131 619 SEA FILE-HCAPLUS ABB-ON PLU-ON 14/RACT
 132 5537 SEA FILE-HCAPLUS ABB-ON PLU-ON 15/RACT
 133 86 SEA FILE-HCAPLUS ABB-ON PLU-ON 16/P
 134 347 SEA FILE-HCAPLUS ABB-ON PLU-ON 17/P
 135 144 SEA FILE-HCAPLUS ABB-ON PLU-ON 18/P
 136 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 136(L)137
 137 12 SEA FILE-HCAPLUS ABB-ON PLU-ON 136 AND 137
 138 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 135(L) (138 OR 139)
 139 10 SEA FILE-HCAPLUS ABB-ON PLU-ON 135 AND (138 OR 139)
 140 20 SEA FILE-HCAPLUS ABB-ON PLU-ON (140 OR 141 OR 142 OR
 141 143)
 142 34845 SEA FILE-HCAPLUS ABB-ON PLU-ON 19
 143 70 SEA FILE-HCAPLUS ABB-ON PLU-ON (135 OR 136) AND 145
 144 4036 SEA FILE-HCAPLUS ABB-ON PLU-ON 19/RACT
 145 50 SEA FILE-HCAPLUS ABB-ON PLU-ON (135 OR 136) AND 147
 146 9 SEA FILE-HCAPLUS ABB-ON PLU-ON 148 AND 144
 147 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 148 AND 144
 148 70 SEA FILE-HCAPLUS ABB-ON PLU-ON 144 OR 146 OR (148 OR
 149 149)
 150 47 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND 150
 151 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND 150
 152 3 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 153 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 154 3 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 155 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 156 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 157 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 158 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 159 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 160 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 161 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 162 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 163 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 164 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 165 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 166 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 167 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 168 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 169 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 170 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)
 171 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND (153 OR 154)

=> dup rem 133 171
 FILE 'CASREACT' ENTERED AT 13:00:44 ON 16 MAY 2007
 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
 COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)
 FILE 'HCAPLUS' ENTERED AT 13:00:44 ON 16 MAY 2007
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGE/TERMS" FOR DETAILS.
 COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)
 PROCESSING COMPLETED FOR 171
 67 DUP REM 133 171 (1 DUPLICATE REMOVED)
 ANSWERS 1-25 FROM FILE CASREACT
 ANSWERS 26-67 FROM FILE HCAPLUS

=> d 174 1-25 1b1b abs fhit

STRUCTURE SEARCH RESULTS

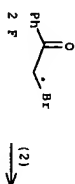
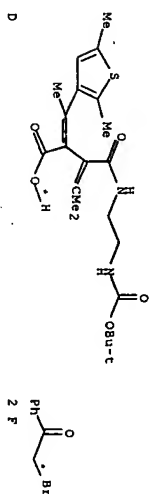
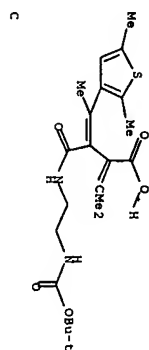
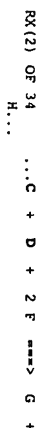
174 ANSWER 1 OF 67 CASREACT COPYRIGHT 2007 ACS ON STN DUPLICATE 1
 ACCESSION NUMBER: 116:6750 CASREACT Full-text
 TITLE: Hydrochlorination of myrcene. Selectivity for
 Cl.
 AUTHOR(S): De Doldan, Griselda V.; Cardell, Daniel; De
 Schilluk, Irma G.
 CORPORATE SOURCE: Inst. Invest. Prod. Nat., IPNAYS, Santa Fe,
 3000, Argent.
 SOURCE: Essence, Derivati Agrumari (1990),
 60(3), 350-7
 CODEN: EDGAMH; ISSN: 0014-0902
 DOCUMENT TYPE: Journal
 LANGUAGE: Spanish
 AB Conditions favoring C(1)-chlorination in the hydrochlorination of β -myrcene were
 examined. The monochloro derivs. were hydrolyzed to the alcs. (geraniol, nerol, etc.),
 which are used in various aromas.



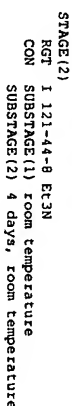
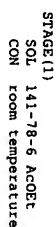
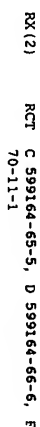
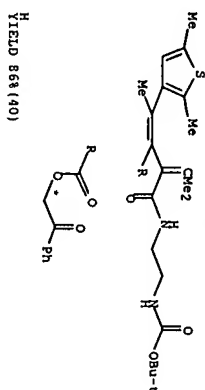
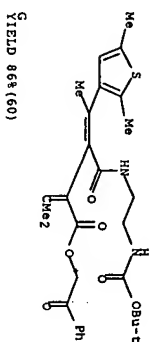
RX(11) RCT I 123-35-3, L 64-19-7
 RGT J 7647-01-0 HCL, D 75-44-5 COC12
 PRO M 16409-44-2

174 ANSWER 2 OF 67 CASREACT COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 139:24508 CASREACT Full-text
 TITLE: Syntheses and UV/VIS properties of
 amino-functionalized polyimides
 AUTHOR(S): Otto, Bernad; Rueck-Braun, Karola
 CORPORATE SOURCE: Institut fuer Chemie, Technische Universitaet
 Berlin, Fakultae II, TC 2, Berlin, 10623,
 Germany
 SOURCE: European Journal of Organic Chemistry (2003), (13), 2409-2417
 PUBLISHER: CODEN: EJOCHF; ISSN: 1434-193X
 DOCUMENT TYPE: Wiley-VCH Verlag GmbH & Co. KGaA
 LANGUAGE: Journal
 English

AB Functionalized fulgimides are regarded as a promising class of photochromic compds. for modulating the structure and function of biomols. A new synthetic route to fulgimides bearing amino-functionalized substituents at the imide N atom was developed. The synthesis of the fulgimides was achieved by base-catalyzed cyclization of phenacyl esters of the succinamic acids derived from fulgides and N-boc-protected allyl- and aryl-substituted diamines with triethylamine or tert-butyl lithium. The UV/visible spectroscopic data and the photochromic properties of these new compds. were studied.

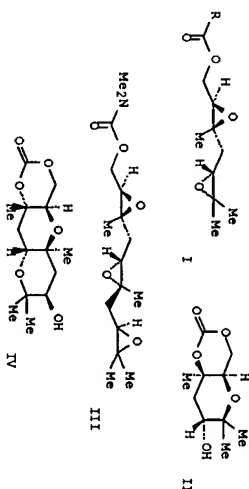


(2)



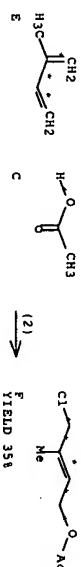
PRO G 599164-67-7, H 599164-68-8
REFERENCE COUNT: 40
THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 3 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 139:117351 CASREACT FULL-TEXT
TITLE: Biomimetic Synthesis of Fused Polypyridine: Oxacyclization Stereo- and Regioselectivity Is a Function of the Nucleophile
AUTHOR(S): Bravo, Fernando; McDonald, Frank E.; Nelvert, Wade A.; Do, Bao; Haddad, Kenneth I.
CORPORATE SOURCE: Department of Chemistry, Emory University, Atlanta, GA, 30322, USA
SOURCE: Organic Letters (2003), 5(12), 2123-2126
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The stereoselectivity of Lewis acid-induced endo-regioselective oxacyclizations of 1,4-diepoxydes is dependent upon the nature of the terminating nucleophile. For instance, ring-opening/recyclization of the carbonate-substituted diepoxide I (R = Me3CO) provides a cis-fused bicyclic product II, whereas carbonate-derived I (R = Me2N) affords the trans-fused diastereomer of II. Stereospecific and regioselective conversion of the tertiary carbonate-terminated 1,4,7-triepoxy III to tricyclic all-trans-fused polypyrans IV is also demonstrated.

RX(2) OF 111 E + C ==> F...



RX(2) RCT E 78-79-5, C 64-19-7

STAGE(1)

RGT B 507-40-4 t-Bu hypochlorite
SOL 64-19-7 AcOH
CON 1 hour, room temperature

STAGE(2)

RGT G 1310-73-2 NaOH
SOL 7732-18-5 Water

PRO F 24529-80-4

NTE stereoselective

42 THERE ARE 42 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L74 ANSWER 4 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 141:350066 CASREACT FULL-TEXT
TITLE: Synthesis and characterization of new chromano
isoxazoles

AUTHOR(S):

Randa, Rami; Rao, Palli, S.; Suryaprabha, R.;
Lakshmi, V. V.; Acharyulu, P. V. N.; Murthy,
Y. L. N.
Dept. of Organic Chemistry, Andhra University,
Visakhapatnam, India

SOURCE:

Chemistry (Rajkot, India) (2003),
1(4), 246-250

CODEN: CHEMCT; ISSN: 0972-8376

PUBLISHER:

Trade Science Inc.

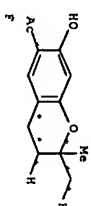
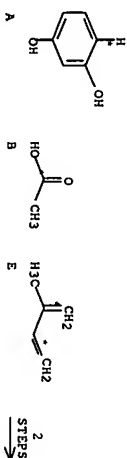
DOCUMENT TYPE:

English

AB The title compds., (five new chromano isoxazoles) were synthesized by condensation of chalcones with hydroxylamine hydrochloride in the presence of alc. KOH. The synthesis involves four steps- Starting with the acylation of Resorcinol using anhydrous ZnCl2 and glacial acetic acid, which afforded Resacetophenone. Resacetophenone was then subjected to nuclear prenylation using isoprene in the presence of polyphosphoric acid and xylene, to form 7-hydroxy-6-acetyl 2,2'-dimethyl chroman. Condensation of Chroman with various substituted benzaldehydes in the presence of alc. KOH furnished different chalcones. Finally, Chalcones were condensed with hydroxylamine hydrochloride in alkaline KOH medium and the title compds. were obtained. Compds. thus obtained were characterized by various spectroscopic techniques to confirm their structures.

RX(13) OF 38 COMPOSED OF RX(1), RX(2)

RX(13) A + B + E ==> F



RX(1) RCT A 108-46-3, B 64-19-7

RGT D 7646-85-7 ZnCl2

PRO C 89-84-9

SOL 64-19-7 AcOH

RX(2) RCT E 78-79-5, C 89-84-9

PRO F 31273-58-2

SOL 1330-20-7 Xylene

NTE polyphosphoric acid used

9 THERE ARE 9 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L74 ANSWER 5 OF 67 CASREACT COPYRIGHT 2007 ACS on STN

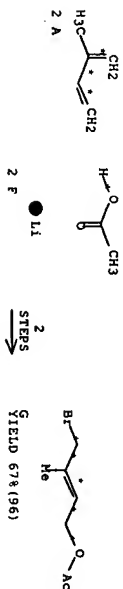
ACCESSION NUMBER: 137:140330 CASREACT Full-text
 TITLE: Process for producing allyl halide compounds
 INVENTOR(S): Doi, Noriyuki; Sato, Shinzo; Kimura, Kazutaka;
 Takahashi, Toshiya
 PATENT ASSIGNEE(S): Japan
 SOURCE: U.S. Pat. Appl. Publ., 8 pp.
 CODEN: USXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002107422	A1	20020808	US 2002-62537	20020205
JP 2002241360	A	20020828	JP 2001-36572	20010214
EP 1231197	A1	20020814	EP 2002-2168	20020129
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003212825	A	20030730	JP 2002-27910	20020205
CN 1373112	A	20021009	CN 2002-107071	20020207
PRIORITY APPL. INFO.:			JP 2001-36570	20010207
			JP 2001-36572	20010214
			JP 2001-349769	20011115
OTHER SOURCE(S): MARPAT 137:140330				



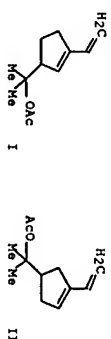
AB Comps. comprising (E)-1,4-dibromo-2-methyl-2-butene and (Z)-1,4-dibromo-2-methyl-2-butene are prepared where the ratio of the E isomer to the total amount of the E and Z isomers is 20:9; a process for producing these compts. and using them to produce an allyl halide compound [I; X = bromine; Y = ASO₂; RCO₂; A = (un)substituted aryl; R = H, lower alkyl, (un)substituted aryl; the wavy line means that the derivative is a mixture of an E or Z geometrical isomer; e.g., (E)-1-(phenylsulfonyl)-3-methyl-4-bromo-2-butene] is described.

RX (7) OF 11 COMPOSED OF RX (1), RX (2)
 RX (7) 2 A + 2 F ==> G + H



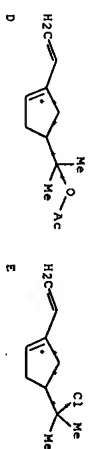
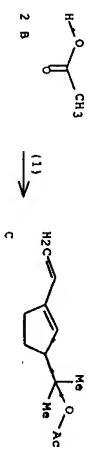
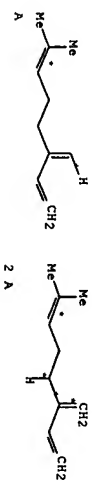
RX (1) RCT A 78-79-5
 RCT D 7726-95-6 B12
 PRO B 16526-19-5, C 16526-18-4
 SOL 25154-42-1 Butane, Chloro-
 RX (2) RCT B 16526-19-5, C 16526-18-4, F 546-89-4
 PRO G 32659-14-6, H 32659-13-5
 SOL 7732-18-5 Water, 68-12-2 DMF

L74 ANSWER 6 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 137:295105 CASREACT Full-text
 TITLE: Palladium catalyzed oxidation of monoterpenes:
 novel oxidation of myrcene with dioxygen
 AUTHOR(S): Goncalves, Jose Alton; Howarth, Oliver W.;
 Gusevskaia, Elena V.
 CORPATE SOURCE: Departamento de Quimica, Universidade Federal
 de Minas Gerais, Belo Horizonte, MG,
 31270-901, Brazil
 SOURCE: Journal of Molecular Catalysis A: Chemical (2002), 185(1-2), 97-104
 CODEN: JMCCEZ; ISSN: 1381-1169
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Myrcene can be efficiently and selectively oxidized by dioxygen in glacial acetic acid containing LiCl, in the presence of the PdCl₂-CuCl₂ catalytic combination, yielding two isomers of a new functionalized monoterpene, i.e., 3-(1-acetoxy-1-methylethyl)-1-vinylcyclopentene (I) and 4-(1-acetoxy-1-methylethyl)-1-vinylcyclopentene (II), as major products. These compts. have a pleasant scent with a flower or fruit tinge and could be used as components of synthetic perfumes. The activities of Pd(OAc)₂-LiNO₃, Pd(OAc)₂-Cu(NO₃)₂ and Pd(OAc)₂-benzoquinone systems in myrcene oxidation have also been examined

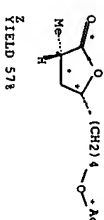
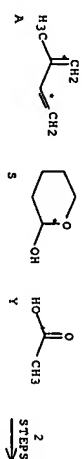
RX (1) OF 1 3 A + 2 B ==> C + D + E



RX(1) RCT A 123-35-3, B 64-19-7
 RGT F 7782-44-7 O2
 PRO C 467449-32-7, D 467449-34-9, E 467449-33-8
 CAT 7647-10-1 PdCl2, 7447-39-4 CuCl2
 SOL 64-19-7 AcOH
 REFERENCE COUNT: 27
 THERE ARE 27 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L74 ANSWER 7 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 136:150747 CASREACT FULL-TEXT
 TITLE: Nickel-catalyzed homomolylation of aldehydes
 in the presence of water and alcohols
 AUTHOR(S): Kimura, Masamichi; Ezoe, Akinori; Tanaka, Shuji; Tamatu, Yoshino
 CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Nagasaki University, Nagasaki, 852-8521, Japan
 SOURCE: Angewandte Chemie, International Edition (2001), 40(19), 3600-3602
 CODEN: ACHIEF; ISSN: 1433-7851
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Aldehydes and cyclic hemiacetals were efficiently homomolylated in presence of Ni(acac)2 and Et3B in THF. The reaction proceeded in reasonable yields with aqueous glutaraldehyde.

RX(15) OF 18 COMPOSED OF RX(7), RX(11)



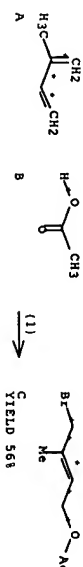
RX(7) RCT A 78-79-5, S 694-54-2
 RGT D 97-94-9 Et3B
 PRO T 394217-74-4
 CAT 3264-82-2 Ni, acetylacetonate
 SOL 109-99-9 THF, 110-54-3 Hexane
 NTE stereoselective, regioselective

RX(11) RCT T 394217-74-4
 STAGE(1)
 RGT AA 10028-15-6 Ozonide
 SOL 75-09-2 CH2Cl2
 STAGE(2)
 RCT Y 64-19-7
 RGT AB 7722-84-1 H2O2
 CAT 7664-93-9 H2SO4
 SOL 64-19-7 AcOH, 7732-18-5 Water
 PRO 2 394217-78-8
 REFERENCE COUNT: 21
 THERE ARE 21 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L74 ANSWER 8 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 134:29587 CASREACT FULL-TEXT
 TITLE: New Synthesis of the Alkaloid Poloniumtoxin C
 AUTHOR(S): Van, T. N.; De Kimpe, N.
 CORPORATE SOURCE: Faculty of Agricultural and Applied Biological Sciences, Department of Organic Chemistry, Ghent University, Ghent, B-9000, Belg.
 SOURCE: Tetrahedron (2000), 56(40), 7965-7973
 CODEN: TETRAH; ISSN: 0040-4020
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Two new short syntheses of the alkaloid poloniumtoxin C were presented. In the first pathway, poloniumtoxin C was obtained in two steps by alkylation of 6-methyl-2,3,4,5-tetrahydro-2-pyridine with (E)-4-bromo-3-methyl-1-(tetrahydro-2-pyran-2-yl)-2-butene and

subsequent deprotection of the THF group. In the second pathway, the cyclic ketimine was constructed via a short sequence of reactions involving first a sequential allylation of the N-(isopropylidene)isopropylamine with N,N-disilylprotected α-bromopropylamine and (E)-4-bromo-3-methyl-1-(tetrahydro-2-pyranloxy)-2-butene, then transamination and deprotection, with the latter two reactions occurring in one step.

RX (1) OF 28 A + B ==> C...



RX (1) RCT A 78-79-5, B 64-19-7

STAGE (1)

RCT D 128-08-5 Bromosuccinimide

SOL 64-19-7 AcOH

STAGE (2)

SOL 7732-18-5 Water

STAGE (3)

SOL 75-09-2 CH2Cl2

PRO C 32659-14-6

NTE STERESELECTIVE

REFERENCE COUNT: 11

THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 9 OF 67 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

130:325271 CASREACT Full-text

TITLE:

Preparation of 8-ocimene] esters for use in

INVENTOR(S):

Sutburg, Horst; Sommer, Horst; Lambrecht,

PATENT ASSIGNEE(S):

Stefan; Woerner, Peter; Guentert, Matthias;

SOURCE:

Haarmann und Reimer G.m.b.H., Germany

DOCUMENT TYPE:

Ger. Offen., 14 pp.

LANGUAGE:

CODEN: GXXBX

FAMILY ACC. NUM. COUNT:

Patent

PATENT INFORMATION:

German

PATENT NO. KIND DATE

DE 19748774 A1 19990506

EP 915079 A1 19990512

EP 915079 B1 20030806

R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE,

MC, PT, IE, SI, LT, LV, FI, RO

ES 2207778 T3 20040601

JP 1126330 A 19990831

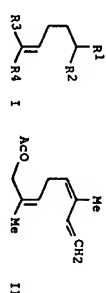
JP 3583933 B2 20041104

US 6034268 A 20000307

US 1998-186267 19981104

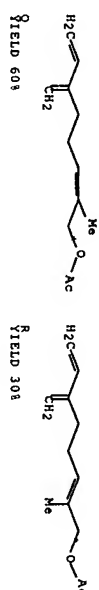
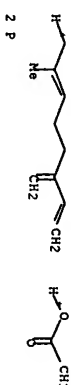
Page 33

PRIORITY APPL. INFO.: DE 1997-19748774 19971105
OTHER SOURCE(S): MARPAT 130:325271



AB Compds. I (R1, R2 = Me, vinyl; R3, R4 = Me, CH2OC6H5; R5 = H, Cl-6-alkenyl, C2-6-alkenyl) are useful as scents and aromatic substances. Thus, (32, 62)-II was prepared from (E/Z)-ocimene via chlorination with NaOCl solution followed by acetylation with NaOAc in DMF containing NaI. (32, 62)-II has a light fresh-green, fruity odor.

RX (4) OF 22 2 P + 2 B ==> Q + R...



RX (4) RCT P 123-35-3

STAGE (1)

RCT J 7681-52-9 NaOCl, K 64-19-7 AcOH

SOL 7732-18-5 Water

STAGE (2)

RCT B 127-09-3

RGT G 7681-82-5 NaI

SOL 68-12-2 DMF

PRO Q 38228-41-0, R 98666-05-8

L74 ANSWER 10 OF 67 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 129:143135 .CASREACT Full-text
TITLE: Diastereoselective azidation of alkenes using 3-acetoxymino-2-(1-hydroxyalkyl)quinazolin-4(3H)-ones in the presence of titanium(IV) tert-butoxide P.; Atkinson, Robert S.; Ayrescough, Andrew P.; Galtrell, W. T.; Raynham, Tony M.; Dep. Chem., Univ. Leicester, LE1 7RH, UK Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1998), (17), 2783-2793 CODEN: JCPR84; ISSN: 0300-922X

AUTHOR(S):
CORPORATE SOURCE:
SOURCE:

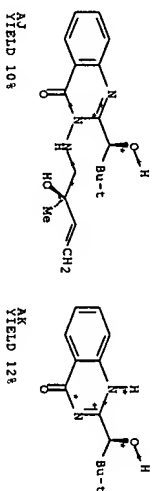
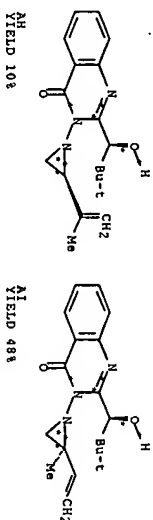
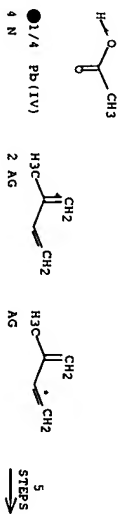
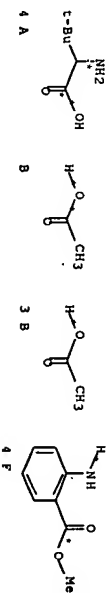
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 3-Amino-2-(1-(S)-1-hydroxy-2-(dimethylpropyl)quinazolin-4(3H)-one 9 (OZNH) was prepared in four steps from (S)-tert-leucine in 43% yield without the need for chromatog. The corresponding 3-acetoxy-aminoquinazolone, prepared in dichloromethane solution by reaction of 9 with lead tetraacetate, reacts with alkenes in the presence of titanium(IV) tert-butoxide to give the corresponding azidines stereoselectively. With styrene and butadiene the corresponding azidines were obtained completely stereoselectively. Indene gave the expected endo-N-invertomer of azidine as the kinetically-formed product (86%) also completely stereoselectively: equilibration to give a 8:1 ratio of exo:endo N-invertomers occurs above 0°C. From an X-ray structure determination one azidine product, the sense of diastereoselectivity in its formation is in agreement with the transition state model. Azidinations of Me acrylate and of tert-Bu acrylate give the resp. products highly stereoselectively (dr:20:1) and with the same sense of diastereoselectivity as identified by an X-ray crystal structure determination previously. Azidinations of α-methylstyrene and Me methacrylate are less completely diastereoselective; isoprene reacts completely diastereoselectively at its unsubstituted double bond but with little diastereoselectivity at its methyl-substituted double bond and the regioselectivity of azidination on the two double bonds is 1.4:1 resp. by comparison to 1.4:7 in the absence of titanium(IV) tert-butoxide.

RX(108) OF 127 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(13)
RX(108) ==> AH + AI + AJ + AK



RX(1) RCT A 20859-02-3, B 64-19-7

STAGE(1)
RCT D 7631-99-4 NaNO3
SOL 64-19-7 AcOH

STAGE(2)
SOL 7732-18-5 Water

PRO C 84621-74-9
NTE STEREOSELECTIVE

RX(2) RCT C 84621-74-9

STAGE(1)
RCT H 68-12-2 DMF, I 7719-09-7 SOCl2
SOL 60-29-7 Et2O

STAGE(2)
RCT F 134-20-3

PRO G 215546-92-2
NTE STEREOSELECTIVE

RX(3) RCT G 215546-92-2

STAGE(1)
RCT L 302-01-2 N2H4
SOL 64-17-5 EtOH

STAGE(2)
SOL 7732-18-5 Water

PRO K 182160-10-7
NTE STEREOSELECTIVE

RX (4) RCT K 182160-10-7, N 546-67-8
 PRO O 182160-08-3
 SOL 865-49-6 CDC13
 RTE STEREOSELECTIVE

RX (13) RCT O 182160-08-3, AG 78-79-5
 PRO AH 215546-97-7, AI 215546-96-6, AJ 215546-98-8, AK
 215546-99-9
 SOL 75-09-2 CH2C12

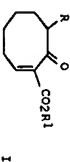
REFERENCE COUNT: 22
 NTE STEREOSELECTIVE
 THERE ARE 22 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L74 ANSWER 11 OF 67 CASREACT COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 127:277975 CASREACT Full-text
 TITLE: Activated cyclooctenones are effective

AUTHOR(S):
 Liu, Hsing-Jang; Wang, Dan-Xiong; Kim, Jeung
 Beaz, Browne, Eric N. C.; Wang, Yu
 Dep. of Chem., Univ. of Alberta, Edmonton, AB,
 T6G 2G2, Can.

SOURCE: Canadian Journal of Chemistry (1997

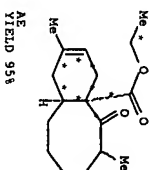
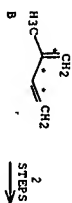
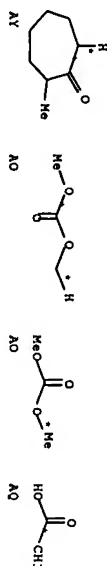
PUBLISHER:
 DOCUMENT TYPE: CODEN: CJCCHG; ISSN: 0008-4042
 National Research Council of Canada
 Journal
 LANGUAGE: English
 GI



1

AB The first Diels-Alder addition of a diene to a cyclooctenone dienophile has been observed. Three activated cyclooctenone dienophiles (I; R = H, R1 = Et; R = R1 = Me; R = Me, R1 = Et) are studied with a variety of simple and functionalized dienes. Diels-Alder adducts are produced in excellent yields under very mild Lewis acid catalyzed conditions. The usual orientation rules are followed, and, as predicted, the products are formed, for the most part, exclusively by ester-endo addition. The stereoselectivity is influenced by the substitution pattern of the diene in some cases. The factors influencing the stereochem. selectivity of the addition are discussed in some detail.

RX (39) OF 56 COMPOSED OF RX (24), RX (17)
 RX (39) AY + 2 AO + AQ + B ----> AE



AE
 YIELD 95%

RX (24) RCT AY 932-56-9, AO 616-38-6

STAGE (1)
 RCT AP 7646-69-7 NaH
 SOL 110-71-4 (CH2OMe)2

STAGE (2)
 RCT AO 64-19-7

STAGE (3)
 RCT AP 7646-69-7 NaH
 SOL 109-99-9 THF

STAGE (4)
 RCT AR 5707-04-0 PhSeCl
 SOL 109-99-9 THF

STAGE (5)
 RCT E 144-55-8 NaHCO3
 SOL 7732-18-5 Water, 60-29-7 Et2O

STAGE (6)
 RCT AL 7722-84-1 H2O2
 SOL 7732-18-5 Water

PRO Y 196398-71-7

RX (17) RCT Y 196398-71-7

STAGE (1)
 RCT D 7705-08-0 FeCl3

SOL 60-29-7 Et2O

STAGE(2)

RCT B 78-79-5

STAGE(3)

RGT E 144-55-8 NaHCO3
SOL 7732-18-5 WaterPRO AE 196398-86-4
REFERENCE COUNT: 24THERE ARE 24 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMATL74 ANSWER 12 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 123:142956 CASREACT Full-textTITLE: Selective transformations of alkynols
catalyzed by ruthenium complexes

AUTHOR(S):

Bruneau, Christian; Kapouche, Zahia; Neveux,
Muriel; Seillier, Benedicte; Dixneuf, Pierre H.
Laboratoire de Chimie de Coordination
Organique, URA CNRS 415, Université de Rennes,
Campus de Beaulieu, Rennes, 35042, Fr.
Inorganica Chimica Acta (1994),
222(1-2), 155-63
CODEN: ICHAA3; ISSN: 0020-1693

SOURCE:

CODEN: ICHAA3; ISSN: 0020-1693
Journal

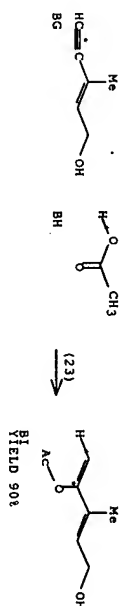
DOCUMENT TYPE:

LANGUAGE:

English

AB Alkynols HC≡C(R)bond CCH2OH, HC≡C(R)bond CCH2CH2OH, and (E)-HC≡C(R)bond CCH=CHCH2OH react with carboxylic acids in the presence of [Ru(μ-O2CH)(CO)2(PH3)]2 to selectively afford keto esters or trisubstituted hydroxy diethyl esters, depending on the possibility of effecting intramol. transesterification. The potential of p-oxopropyl esters as mild acylating reagents and precursors of hydroxy amides, dipeptides, pseudodipeptides, polycarbonyl compds., and acetylenic 1,2-diols has been shown.

RX(23) OF 30 BG + BH ==> BI



RX(23) RCT BG 6153-06-6, BH 64-19-7

STAGE(1)

CAT 151516-73-3 Ruthenium, tetracarbonylbis(μ-
(formate-KO:K'O'))bis(triphenylphosphine).
(dl-, (Ru-Ru))

SOL 108-88-3 PhMe

STAGE(2)

RGT D 144-55-8 NaHCO3

PRO BI 166945-58-0

L74 ANSWER 13 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 116:214034 CASREACT Full-text

TITLE:

Enantioselective synthesis of cyclopentanoid

AUTHOR(S):

compounds from isoprene and diperylene
Baldenius, Kai U.; Tom Dieck, Heindrik;
Koenig, Wilfried A.; Icheln, Detlef; Runge,
Torsten

CORPORATE SOURCE:

Inst. Anorg. Angew. Chem., Univ. Hamburg,
Hamburg, W-2000/13, Germany

SOURCE:

Angewandte Chemie (1992), 104(3),
338-40 (See also Angew. Chem., Int. Ed. Engl.,
1992, 31(3), 305-7)

DOCUMENT TYPE:

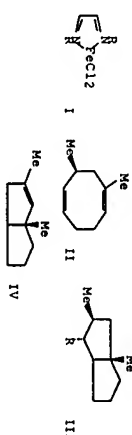
CODEN: ANCEAD; ISSN: 0044-8249

LANGUAGE:

Journal

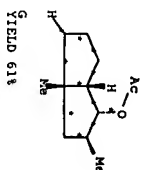
GI

German



AB Cyclization of isoprene with piperylene in the presence of complex I (R = (1R)-menthyl) and butadienemagnesium-2 Tiff gave 90% cyclooctadiene II, ee = 61%. Isomerization of II in the presence of an acid catalyst such as BF3·Et2O and an agent such as AcOH or PhH gave bicyclo compds. such as III (R = OAc, Ph) and IV.

RX(5) OF 7 COMPOSED OF RX(1), RX(2)
RX(5) A + B + F ==> G



RX (1) RCT A 78-79-5, B 2004-70-8

PRO C 138541-38-5
CAT 87226-78-6 Iron, dichloro[N,N'-1,2-ethanediylidenebis(5-methyl-2-(1-methylethyl)cyclohexanamine)-N,N'-1-],

[7-4-[1R-[1a(1'R,2'S,5'R'),2b,5a]]]-,

83995-88-4 Magnesium, 2-butene-1,4-diybis(tetrahydrofuran)-, (T-4)-

NTE stereoselective

RX (2) RCT C 138541-38-5, F 64-19-7

RGT H 7664-93-9 H2SO4

PRO G 138541-39-6

SOL 64-19-7 AcOH

NTE stereoselective

L74 ANSWER 14 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 116:20816 CASREACT Full-textTITLE: Pigments of Fungi. XXI. Synthesis of
(±)-6-demethoxyaustrocortilubin

AUTHOR(S): Burns, Christopher J.; Gill, Melvyn; Saubern, Simon

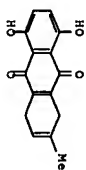
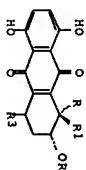
CORPORATE SOURCE: Sch. Chem., Univ. Melbourne, Parkville, 3052, Australia

SOURCE: Australian Journal of Chemistry (1991), 44(10), 1427-45

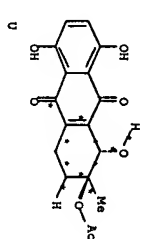
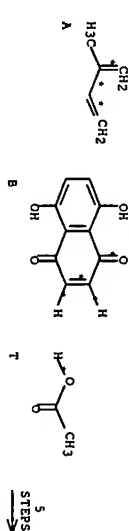
DOCUMENT TYPE: CODEN: AJCHAS; ISSN: 0004-9425

LANGUAGE: English

GI



AB 6-Demethoxyaustrocortilubin (I, R-R2 = H), is synthesized via the epoxide I (RR2 = bond, R1, R3 = H) which is available in 73% yield over four steps from naphthazarin. Hydrolysis of I (RR2 = bond, R1, R3 = H) yields the diol I (R, R2, R3 = H, R1 = OH) which on hydrogenolysis affords 6-demethoxy-1-deoxyaustrocortilubin (I, R-R3 = H). Stereoselective benzylic hydroxylation of (I, R-R3 = H) gives I (R-R2 = H, R3 = OH). Cleavage of I (RR2 = bond, R1, R3 = H) with AcOH-AcOH affords a mixture of the esters I (R = OAc, R1-R3 = H, R = OH, R1, R3 = H, R2 = Ac; R = R2 = R3 = H, R1 = OH), while methanolysis yields I (R = R2 = R3 = H, R1 = OMe) and its isomer. Hydrogenolysis of I (R = R2 = R3 = H, R1 = OAc, OMe; R = OH, R1 = R3 = H, R2 = Ac) gives high yields of I

RX (55) OF 62 COMPOSED OF RX (1), RX (3), RX (10), RX (11), RX (12)
RX (55) A + B + T ==> U

RX (1) RCT A 78-79-5, B 475-38-7

PRO C 14569-43-8

RX (3) RCT C 14569-43-8

RGT F 1310-73-2 NaOH

PRO E 65698-32-0

NTE H(+)

RX (10) RCT E 65698-32-0

RGT R 1493-13-6 F3CSO2H

PRO H 137788-35-3

RX (11) RCT M 137788-35-3

RGT H 937-14-4 MCPBA

PRO S 137788-36-4

RX (12) RCT S 137788-36-4, T 64-19-7

PRO U 137788-37-5

L74 ANSWER 15 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 111:194066 CASREACT Full-text

TITLE: Acyloxyhalogenation of 1,3-diene hydrocarbons

AUTHOR(S): Ivanov, S. V.; Stadenchuk, M. D.

CORPORATE SOURCE: Leningr. Tekhnol. Inst., Leningrad, USSR

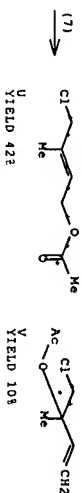
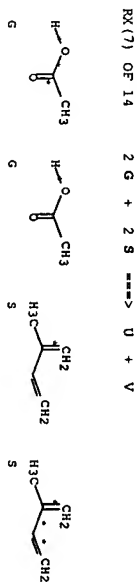
SOURCE: Zhurnal Obshchei Khimii (1989), 59(4), 865-73

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB
Acryloyloxylation of divinyl with p-ClC₆H₄SO₂NaCl₂ in HCO₂H, AlCl₃, Me₂SO, CH₂Cl₂ led to the resp. 1,2- and 1,4-addition products ClCH₂CH=CHCH₂O₂CH₂Cl and ClCH₂CH(OCH₂CH=CH₂)CH₂Cl in comparable yields (i.e., 56:44 for R = H). t-BuCO₂H was found to suppress the competing polymerization reaction, and enhances the 1,4-addition reaction. Acryloylaldehyde of isoprene and CH₂=CMeCH=CH₂ was also studied. The authors warn of the possibility of explosion in the direct distillation of products from the reaction mixture, as well as the allergic nature of the reaction products.



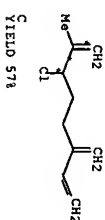
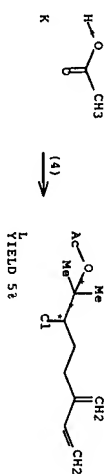
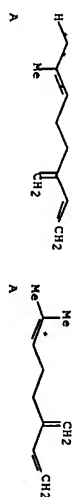
RX (7)	
RCR	G 64-19-7, S 78-79-5
RCF	E 17260-65-0, Benzene sulfonamide, N,N, 4-trichloro-, F
	7791-03-3, LiClO4
PRO	U 38872-49-0, V 24517-68-8
SOL	64-19-7 AcOH

L74 ANSWER 16 OF 67
 CASREACT COPYRIGHT 2007 KGS ON STN
 ACCESSION NUMBER: 112:36192 CASREACT FULL-TEXT
 TITLE: Formal ene-chlorination of mycene by
 N-chlorosuccinimide
 AUTHOR(S): Schütz, Klaus; Hauke, Günter; Koehler,
 Günter
 Sekt. Chem., Karl-Marx-Univ., Leipzig,
 DDR-7010, Ger. Dem. Rep.
 Zeitschrift fuer Chemie (1989),
 CORPORATE SOURCE:
 SOURCE:

DOCUMENT TYPE: Journal

LANGUAGE: German

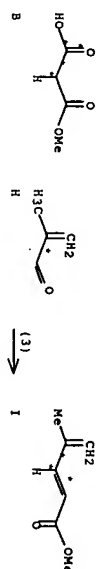
AB Reaction of myrcene with NCS in ROH (R = H, Me, Ac) containing H₂SO₄ gave Me₂C(OBRC)CHC(CH₂CH₂C)(CH₂)CH:CH₂ in 64, 38, and 35 yields, resp., along with 21-57% CH₂:C(CH₂CH₂C)CH₂:CHC(CH₂)CH:CH₂ (I). I reacted with KSCN or NaOAc (R1 = H, Ac, CH₃O) to give 44-60% CH₂:CMeCH₂CH₂CH₂C(CH₂)CH:CH₂ (R2 = SCN, R1).



RX(4)
 RCT A 123-35-3, K 64-19-7
 RGT D 128-09-6 Chlorosuccinimide
 PRO L 124331-86-3, C 72420-53-2
 CAT 7664-93-9 H2SO4
 SOL 64-19-7 AcOH

AUTHOR(S): RODRIGUEZ, J.; WAGGELL, B.
CORPORATE SOURCE: Fac. Sci., Stirling, Univ. Aix-Marseille III, Marseille, F-13397, F-134-5
SOURCE: Synthesis, 1988, (7), 1029-1081

DOCUMENT TYPE:	Journal
LANGUAGE:	English
AB	<p>α,β-Unsaturd. aldehydes reacted with monoalkyl malonate and pyridine with a catalytic amt of DMAP in a regio- and stereoselective process to yield almost exclusively 2,4-<i>trans</i>-chromophoric esters with essentially (and in many cases exclusively) the 2<i>E</i>-stereochrom. Thus, HO2CC(CH2O)2Me and RCH=CR1CHO (R = H, Me, Ph, R1 = H, R = H, R1 = Me; R1 = CH3CHO) gave 84-100% RCH=CHCH=CHCO2Me.</p>



RX(3) RCT B 16695-14-0, H 78-85-3
RGT D 1122-58-3, 4-DMAF
PRO I 37974-16-6
SOL 110-86-1 Pyridine

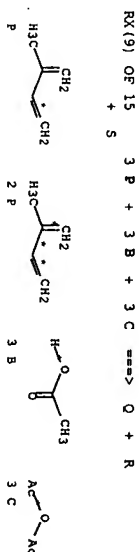
L74 ANSWER 18 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 103:5870 CASREACT Full-text
TITLE: Liquid-phase 1,4-diacetoxylation of conjugated
diene with tellurium(IV) oxide and alkali
metal halides

AUTHOR(S): Uemura, Sakae; Fukuzawa, Shinichi; Patil,
Suresh R.; Okano, Masaya
CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Kyoto, 611,
Japan

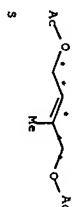
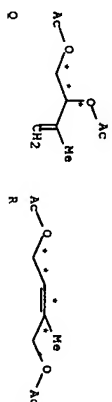
SOURCE: Journal of the Chemical Society, Perkin
Transactions 1: Organic and Bio-Organic
Chemistry (1972-1999) (1985), (3),
499-503
CODEN: JCPR84; ISSN: 0300-922X

DOCUMENT TYPE: English
LANGUAGE: English

AB Oxidation of CH₂=C(R)CH=CH₂ (R = H, Me; R = H, Me) with TeO₂ in HOAc
containing LiBr gave isomeric mixts. of the corresponding diacetoxyalkene 1,2- and 1,4-
addition products; the product yields and selectivities were high in the presence of
excess LiBr. The reaction also occurred in the presence of NaBr, KBr, LiCl, HBr, or
Iodine, but yields and selectivities were lower. The mechanism is discussed.



(9)



RX(9) RCT P 78-79-5, B 64-19-7, C 108-24-7
RGT G 7446-07-3 TeO₂, H 7550-35-8 LiBr
PRO Q 30264-53-0, R 59055-00-4, S 59054-99-8

L74 ANSWER 19 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 98:142973 CASREACT Full-text
TITLE: 4-Chloro-3-methylcrotyl esters
Dalippon Ink and Chemicals, Inc., Japan;
PATENT ASSIGNEE(S): Kawamura Physical and Chemical Research
Institute

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF

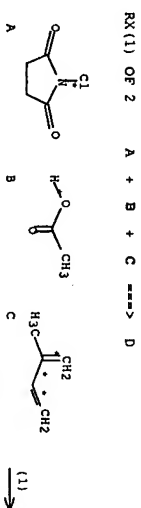
DOCUMENT TYPE: Patent

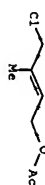
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 57183742	A	19821112		
PRIORITY APPLN. INFO.:				
JP 1981-65238		19810501		
AB RCO ₂ CH ₂ CH:CHCH ₂ Cl (I; R = alkyl, aralkyl, Ph) were prepared by esterification of RCO ₂ H with isoprene and chlorinating agents. Thus, 18 g N-chlorosuccinimide was dissolved in 36 g HOAc at 45°, 13 g isoprene in HOAc added at 45-55°, and the solution heated at 50-55° to give 4.5 g trans-I (R = Me) and 3.0 g MeCO ₂ CH ₂ CH:CHCH ₂ Cl.				





D

RX (1) RCT A 128-09-6, B 64-19-7, C 78-79-5
PRO D 38872-49-0

L74 ANSWER 20 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 97:91789 CASREACT Full-text
TITLE: Stereospecific palladium-catalyzed
1,4-acetoxychlorination of 1,3-dienes
AUTHOR(S): Baerckvall, Jan E.; Nordberg, Ruth E.;
Nyström, Jan E.
CORPORATE SOURCE: Dep. Org. Chem., R. Inst. Technol., Stockholm,
S-100 44, Sweden.
Tetrahedron Letters (1982), 23(15),
1617-20

SOURCE: CODEN: TETLEY; ISSN: 0040-4039

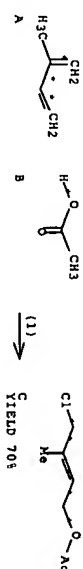
DOCUMENT TYPE: Journal
LANGUAGE: English

G1



AB Pd-catalyzed oxidation of cyclic and acyclic 1,3-dienes in AcOH in the presence of LiCl/LiOAc gave 1-acetoxy-4-chloro-2-alkenes with high selectivity. E.g., addition of cyclohexa-1,3-diene to a mixture of benzoinone, Pd(OAc)₂, and LiCl/LiOAc in AcOH over 3 h, followed by reaction at room temperature for 5 h, gave 89% of a >98:2 mixture of cyclohexenes I (R = β-, α-Cl, R1 = OAc). The mechanism involves π-allyl complex formation through (E)-acetoxy-palladation of 1 double bond followed by external (E)-attack by Cl-. The 1,4-adducts were stereo- and regioselectively functionalized. E.g., substitution reaction of I (R = β-Cl, R1 = OAc) with Me₂NH gave 93% I (R = α-Me₂N, R1 = OAc), which underwent substitution reaction with NaCH(CO₂Me)₂ to give 80% I (R = α-Me₂N, R1 = CH(CO₂Me)₂).

RX (1) OF 19 A + B ==> C...



RX (1) RCT A 78-79-5, B 64-19-7
PRO C 38872-49-0

CAT 106-51-4 p-Benzquinone

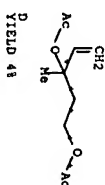
L74 ANSWER 21 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 98:71424 CASREACT Full-text
TITLE: Ruthenium-catalyzed Prins reaction
AUTHOR(S): Thivolle-Cazat, Jean; Trachtenko, Igor
CORPORATE SOURCE: Inst. Rech. Catal., Villeurbanne, 69626, Fr.
Journal of the Chemical Society, Chemical
Communications (1982), (19), 1128-9
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The preparation of 1,3-diol derivs. by the Prins reaction of dienes and alkenes with aldehydes and carboxylic acids was catalyzed by Ru salts. E.g., reaction of (H₂C=CH)₂ (I) with paraformaldehyde and MeCO₂H in the presence of RuCl₃ in the absence of solvent for 20 h gave a 5:23:10 mixture of 4-vinyl-m-dioxane (II) and H₂C=CHCH(OAc)(CH₂)₂OR (III); R = H, Ac) together with 17 parts oligomeric H₂C=CHCH(OAc)CH₂CH₂CH₂CH₂CH₂OR (IV). The ratio of cyclic product to oligomer varied with the reaction conditions. E.g., similar reaction in the presence MeONa for 20 h gave a 2.5:39.6:24 mixture of II, III (R = H, Ac), and IV.

RX (1) OF 1 A + B + C ==> D



YIELD 48

RX (1) RCT A 78-79-5, B 50-00-0, C 64-19-7
PRO D 80118-03-2

L74 ANSWER 22 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 97:145026 CASREACT Full-text
TITLE: Syntheses of dihydrolawandiol and its related compounds from carboxylic acids and conjugated dienes
AUTHOR(S): Fujita, Tsutomu; Watanabe, Shoji; Suga, Kyoichi; Maeda, Toshio; Suganaka, Kotoji; Kikuchi, Hajime
CORPORATE SOURCE: Dep. Appl. Chem., Chiba Univ., Chiba, 260, Japan

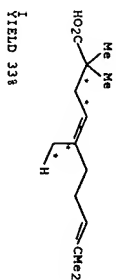
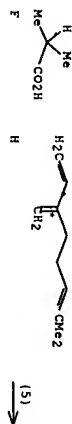
SOURCE: Journal of Chemical Technology and Biotechnology (1979-1982) (1982), 32(3), 476-84
CODEN: JCTBDC; ISSN: 0142-0356



DOCUMENT TYPE: Journal
LANGUAGE: English

AB Slow addition of isoprene in THF to 3-methylbutanoic acid, Me₂NCN:CHMe₂, and Na naphthalenide in THF under N at room temperature followed by refluxing 8 h and standing overnight gave 658 dihydroxylavandilic acid (I), LIAIH₄ reduction of which gave 858 title compound MeC:CHCH₂CH(CH₂OH)CHMe₂ (II). II is used in com. fragrances. Oxidation of II with pyridinium chlorochromate gave 818 dihydroxylavandilaldehyde (III). Cyclization of I with H₂SO₄ in C₆H₆ gave 828 5,5-dimethyl-2-isopropyl-6-valerolactone (IV). Several analogs of I-IV were prepared similarly. 2-Alkyl- and 2,2-dialkyl-substituted 5-methyl-4-hexenols, 5-methyl-4-hexenals, and 5,5-dimethyl-5-pentanolides have sweet odors and can be used in perfumes.

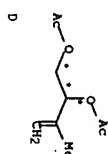
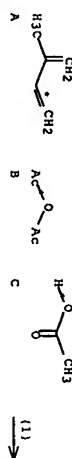
RX (5) OF 103 F + H ==> I



RX (5) RCT F 79-31-2, H 123-35-3
PRO I 70777-58-1

L74 ANSWER 23 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 95:199042 CASREACT Full-Text
TITLE: Selective 1,4-diacetoxylation of conjugated dienes with tellurium(IV) oxide
AUTHOR(S): Uemura, Sakae; Fukuzawa, Shinichi; Okano, Masaya
CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Kyoto, 611, Japan
SOURCE: Tetrahedron Letters (1981), 22(52), 5331-4
CODEN: TELENY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Oxidation of linear conjugated dienes with TiO₂ and LiBr in AcOH gave a mixture of 1,2- and 1,4-diacetoxyalkenes. When the ratio of LiBr to TiO₂ was 5-10 the 1,4-isomer was produced highly selectively. E.g., reaction of 5 equiv butadiene with AcOH-Ac₂O, 1 equiv TeO₂, and 5 equiv LiBr at 125° for 20 h gave a 1:9 mixture of CH₂:CHCH(OAc):CH₂OAc and (E)- and (Z)-AcOCH₂CH:CHCH₂OAc.

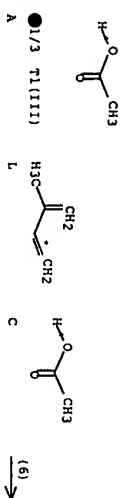
RX (1) OF 6 A + B + C ==> D

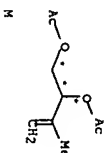


RX (1) RCT A 78-79-5, B 108-24-7, C 64-19-7
RCT E 7446-07-3 TeO₂, F 7550-35-8 LiBr
PRO D 30264-53-0

L74 ANSWER 24 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 95:96978 CASREACT Full-Text
TITLE: Diacetoxylation of conjugated dienes with thallium(III) acetate in acetic acid
AUTHOR(S): Uemura, Sakae; Miyoshi, Haruo; Tabata, Akira; Okano, Masaya
CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Kyoto, 611, Japan
SOURCE: Tetrahedron (1981), 37(12), 291-5
CODEN: TETRAH; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Conjugated dienes reacted with Tl(OAc)₃ in AcOH to give isomeric mixts. of the 1,2- and 1,4-diacetoxyalkene addition products. 1,2-Addition products predominated. E.g., CH₂:CHMe:CH₂ reacted with Tl(OAc)₃ (AcOH, 20°, 1 h) to give 71% of an 83:17 mixture of CH₂:CHMe:CH₂OAc and AcOCH₂CH:CHMe:CH₂OAc. The mechanism of the reaction is discussed.

RX (6) OF 11 A + L + C ==> M





EX(6) RCT A 2570-63-0, L 78-79-5, C 64-19-7
PRO M 30264-53-0
CAT 108-24-7 Ac2O

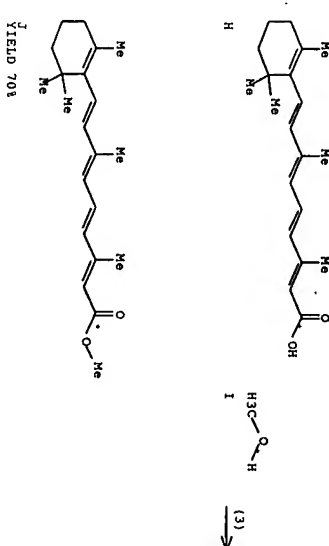
L74 ANSWER 25 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 57:29494 CASREACT Full-text
TITLE: Synthesis of carboxylic acid esters by the imidazole method
AUTHOR(S): Stebb, Heinz A.; Manschreck, Albrecht
CORPORATE SOURCE: Univ. Heidelberg, Germany
CHEMISCHER SOURCE: Chemische Berichte (1962), 95, 1284-97
CODEN: CHEMAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

The basecatalyzed imidazole method allowed the preparation of esters from carboxylic acids and alcs. at room temperature in extremely short reaction periods with very good yields. The new method was applied to the prepn. of esters from highly unsatd. alcs. and carboxylic acids of the vitamin A series and the prepn. of esters of tart-alcs. Starting from N,N'-carbonyldimazole (I), sym. and unsym. esters of carboxylic acids were obtained, as well as imidazole-N-carboxylic acid esters, the pyrolysis of which yielded N-substituted imidazoles. Adipic acid dimidazolid (12.31 g.) (from equimolar amts. of adipic acid and I in tetrahydrofuran) treated at room temperature with stirring with 0.015 g. Na in 60 cc. absolute MeOH, the mixture treated after 0.5 min. with 17 cc. 6.2N HCl, evaporated in vacuo, and the residue extracted with Et2O yielded 7.35 g. (CH2CHCO2Me)2, b12.5-13.12.5°, n20D 1.4285. PCH2OH (21.02 g.) in 70 cc. THF, refluxed with 0.20 g. Na, added at 20° to 33.73 g. N-benzoylimidazole (II) in 60 cc. THF, evaporated after 1 h., the residue kept several hrs. with 80 cc. H2O and 80 cc. Et2O, and the extract worked up yielded 36.0 g. BzOCH2Ph (III), m. 1920°, b13 180-1°. Na (0.20 g.) and 2.0 g. imidazole in 20 cc. THF refluxed, cooled, treated with 21.02 g. PCH2OH in 50 cc. THF, and processed in the usual manner yielded 34.1 g. III. I (27.88 g.) in 200 cc. THF stirred 2 h. at room temperature with 20.0 g. BzOH and treated with a solution of 0.17 g. Na and 18.60 g. PCH2OH in 80 cc. THF gave in the usual manner 30.7 g. III. N-Acetylimidazole (16.75 g.) in 150 cc. THF mixed with 19.70 g. PCH2OH in 50 cc. THF, kept overnight, evaporated, the residue shaken with the 3-fold amount of H2O, and extracted with Et2O yielded 20.25 g. PCH2OHCH2OMe, b15 139-41.5°, n20D 1.3428. PCH2OH in 30 cc. THF added at room temperature to 0.40 g. Na and 4.0 g. imidazole in 40 cc. THF, the mixture treated with 21.25 g. II in 30 cc. THF, kept overnight, and worked up gave 22.75 g. PCH2OHCH2OMe, m. 39-9.5°, b0.1 137-8.5°. I (19.89 g.) in 100 cc. THF stirred 2 h. with 14.30 g. BzOH and added at room temperature to 0.40 g. Na, 4.0 g. imidazole, and 15.71 g. PCH2OH in 80 cc. THF, added at room temperature to 0.10 g. Na and 2.0 g. imidazole dissolved in 25 cc. THF, the mixture treated with 7.10 g. N-palmitoylimidazole in 100 cc. THF, kept at room temperature overnight and some time at 50°, evaporated, the residue ground with 250 cc. N NaOH kept 6 h., filtered, and the filtrate worked up yielded 6.19 g. C15H31O2N2CH2CH2OH, leaflets, m. 46-6.5° (EtOH). PCH2OHCH2OMe (14.08 g.) in 150 cc. THF stirred 1 h. with 16.20 g. I, treated with 0.46 g. Na in 5.0 g. MeOH, evaporated after 1 h., the residue shaken with 200 cc. H2O, and the aqueous solution extracted with Et2O yielded 11.05 g. PCH2OHCH2OMe, m. 34-5.5°, b15 132.5-34°. Na (0.05 g.) and 1.0 g. imidazole in THF under N treated successively with 2.20 g. N-acetylimidazole in 80 cc. THF and 2.91 g. vitamin A (IV) in 27 cc. THF, stirred 2 h., evaporated, the residue kept with H2O overnight, extracted with Et2O, and the extract worked up yielded 2.17 g.

pale yellow acetate of IV, m. 57-9°. Vitamin A acid (V) (2.37 g.) in 50 cc. C6H6 stirred 4 h. with 1.34 g. I, refluxed a few min., evaporated, the residue dissolved in 45 cc. absolute MeOH under N, treated with 0.18 g. Na in 15 cc. MeOH, kept overnight, filtered, evaporated, the residue shaken with 200 cc. H2O, and refrigerated overnight yielded 2.25 g. Na ester of V, pale yellow needles, m. 55-5.6.5° (6:1 MeOH-H2O). V (3.55 g.) and 3.14 g. I processed in the usual manner, the residue dissolved in absolute EtOH, treated with 0.20 g. Na in 30 cc. EtOH, kept overnight, diluted with 150 cc. H2O, shaken occasionally during 5 h., extracted with petr. ether, and the extract worked up gave 5.37 g. Et ester of V, yellow oil, b0.6 180°. IV (3.21 g.) in 50 cc. THF treated with 0.05 g. Na and 1.0 g. imidazole in 50 cc. THF, the mixture treated with 3.93 g. imidazolidine of V in 100 cc. THF, diluted after 5 h. with 80 cc. H2O, kept overnight, evaporated, and the residue extracted with 200 cc. petr. ether yielded 4.62 g. IV ester of V, orange oil; all operations were conducted under N. N-Palmitoylimidazole (4.57 g.) and 2.62 g. L-ascorbic acid in 150 cc. HCONH2 kept overnight under N, evaporated at 70° in vacuo, and recovered, from Me2CO yielded 1.23 g. 3-palmitoyl-L-ascorbic acid, m. 95-6°. Na (0.23 g.) dissolved in 30.0 g. Me3COH, cooled, added dropwise to 11.82 g. III, diluted with 20 cc. THF, kept overnight, evaporated, the residue kept 3 h. with 50 cc. H2O and 50 cc. Et2O, and the Et2O phase worked up yielded 10.38 g. Me3COH (VI), b0.9 52.5-53°, n20D 1.4908. I (20.0 g.) in 40 cc. THF stirred 1 h. with 14.30 g. BzOH, mixed with 0.45 g. Na in 30.0 g. Me3COH, and worked up yielded 19.0 g. VI. N-(p-tert-butylbenzoyl)imidazole (9.87 g.) in 35 cc. Me3COH and 15 cc. THF added to 0.20 g. Na in 35 cc. Me3COH, kept at 33° overnight, diluted with 150 cc. H2O, stirred 4 h., evaporated, and extracted with Et2O yielded 7.58 g. p-Me3CO6H4CO2CH3, b15 152.5-3.5°, n20D 1.4904. Na (0.23 g.) in 23 cc. hot Me3COH cooled to 40°, treated with 18.76 g. isobutyric acid imidazolidine, kept overnight, distilled, the residue shaken with H2O, extracted with Et2O, and the extract worked up yielded 13.6 g. 150-PCO2CHMe3, b. 127-9°, n20D 1.3928. Na (0.30 g.) in 30 cc. Me3COH and 25 cc. THF treated with 8.7 g. trimethylacetylimidazolidine in 10 cc. THF, kept overnight, distilled, and the residue worked up with H2O and Et2O yielded 5.74 g. Me3COCH3, b. about 125°. n20D 1.3925. N-Acetylimidazole (12.54 g.) in 140 cc. THF and 30 cc. Me3COH added at 50° to 2.28 g. Na in 184 cc. Me3COH, stirred 1 h., and filtered yielded 7.0 g. Na dehydracetate; an aqueous solution of the salt treated dropwise with cooling with concentrated H2SO4 yielded 308 dehydracetic acid, m. 108-10° (aqueous EtOH). N-Propionylimidazole (12.0 g.) in 20 cc. THF treated with 0.25 g. Na in 16.5 g. Me3COH, kept 40 h. at 33°, neutralized with 100 cc. 0.1N HCl, and extracted with Et2O yielded 5.45 g. (crude) EtCOCHMeCO2CHMe3, b15 92.5-4.5°, n20D 1.4224, green with FeCl3 in MeOH; a sample boiled with concentrated HCl in EtOH and treated with 2,4-(O2N)2C6H3NH2 gave 2,4-(O2N)2C6H3NHNH2CEt2, m. 152.5-4.5°. I (12.73 g.) in 20 cc. THF treated with 0.15 g. Na and 16.22 g. PCH2OH in 80 cc. THF, stirred 2.5 h., evaporated, and refrigerated yielded 15.9 g. CO(CH2Ph)2, m. 29-9.5°, n20D 1.5451. Na (0.29 g.) in 28 cc. Me3COH and 10 cc. THF added dropwise during 2 h. to 21.18 g. I in 200 cc. THF, kept overnight, evaporated, diluted with H2O, and extracted with Et2O yielded 15 g. N-carbo-tert-butylimidazole (VIII), m. 45-7.5° (petr. ether). VII heated at 160-70° evolved CO2; the residue consisted of imidazole, Na (0.17 g.) in 19 cc. Me3COH added at 50° to 8.60 g. I in 22 cc. THF, kept overnight, refluxed 6 h., distilled, the residue treated with H2O, and refrigerated gave 4.85 g. CO(CHMe3)2, m. 58.5-40.5° (aqueous EtOH). Na (0.10 g.) in 2.4 cc. EtOH added to 6.8 g. VII in 0.8 cc. EtOH, kept at room temperature overnight, diluted with H2O, and extracted with Et2O yielded 4.5 g. CO(CHMe3)2, b. 139-41°, n20D 1.3947. EtOH (3.13 g.) added slowly dropwise to 11.02 g. I in 170 cc. THF, heated 1.5 h. at 50°, evaporated, the residue kept 45 min. at room temperature with 200 cc. dry CCl4, filtered, and distilled gave 6.8 g. N-carbomethoxyimidazole (VIII), b16-17 105-7°, n20D 1.4760. Imidazole with ClCO2Et also gave VIII, b15 101.5-4.5°, n20D 1.4763. PCH2OH (12.50 g.) containing 0.40 g. Na added dropwise to 19.7 g. I in 200 cc. THF, stirred 1 h. at 30°, evaporated, the residue kept some time at 20-30° in vacuo, diluted with 30 cc. dry CCl4, filtered, and the filtrate worked up gave 18.5 g. reddish oily N-carbomethoxyimidazole (IX), n20D 1.5476. Crude IX (16.28 g.) distilled in vacuo yielded 4.21 g. N-benzoyl-imidazole (X), m. 70-2° (petr. ether). ClCOCH2Ph (10.45 g.) and 8.34 g. imidazole heated 0.5 h. with stirring at 100° and diluted with 200 cc. dioxane precipitated 7.0 g. X, m. 68-70°. IX (11.33 g.) and 4.0 cc. EtOH heated 2 h. at 40-50°, kept overnight, diluted with 50 cc. H2O, and extracted after 2 h. with Et2O yielded 5.96 g. EtCOCH2CH2Ph (XI), b0.1 66-71°, m. 69.5-72° (petr. ether). VIII (21.85 g.) and 16.84 g. PCH2OH in 20 cc. THF heated 3 h. at 80°, kept overnight, and worked up yielded 13.9 g. XI, b15 126-30°, n20D 1.4913. Na (0.58 g.) in 13.50 g. PCH2OH and 20 cc. THF added to 19.45 g. VIII, kept overnight, and worked up in the usual manner yielded 9.1 g. XI, b15 129-33°, n20D 1.4919, and 5.7 g. CO(CH2Ph)2, b15 205-7°, m. 21-3°.

RX(3) OF 5 H + I -> J



RX(3) RCT H 302-79-4, I 67-56-1
 RGT F 530-62-1 Dimethylol ketone
 PRO J 339-16-2
 SOL 71-43-2 Benzene, 67-56-1 MeOH
 NTE Classification: Esterification; Alkoxylation; #
 Conditions: carbodimazole, benzene 4h; several mm Rf;
 NaOMe MeOH; overnight/NZ

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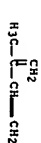
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174 ANSWER 26 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:760441 HCAPLUS Full-text
 DOCUMENT NUMBER: 140:63804
 TITLE: Protocol for the development of the master
 chemical mechanism, MCM v3 (part h):
 tropospheric degradation of non-aromatic
 volatile organic compounds
 Saunders, S. M.; Jenkin, M. E.; Derwent, R.
 G.; Pilling, M. J.
 School of Chemistry, University of Leeds,
 Leeds, LS2 9JT, UK
 Atmospheric Chemistry and Physics (2003), 3(1), 161-180
 CODEN: ACPTCE; ISSN: 1680-7324
 PUBLISHER: European Geophysical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

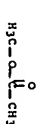
ED Entered STN: 29 Sep 2003
 AB Kinetic and mechanistic data relevant to the tropospheric degradation of volatile organic compounds (VOC), and the production of secondary pollutants, were previously used to define a protocol which underpinned the construction of a near-explicit Master Chemical Mechanism. An update to the previous protocol is presented, which was used to

define degradation schemes for 107 nonarom. VOC as part of version 3 of the Master Chemical Mechanism (MCM v3). The treatment of 18 aromatic VOC is described in a companion paper. The protocol is divided into subsections describing initiation reactions, the reactions of the radical intermediates and the further degradation of 1st and subsequent generation products. Emphasis is placed on updating the previous information, and outlining the methodol. which is specifically applicable to VOC not considered previously (e.g., α - and β -pinene). The present protocol aims to take into consideration work available in the open literature up to the beginning of 2001, and some other studies known by the authors which were under review at the time. Application of MCM v3 in appropriate box models indicates that the representation of isoprene degradation provides a good description of the speciated distribution of oxygenated organic products observed in reported field studies where isoprene was the dominant emitted hydrocarbon, and that the α -pinene degradation chemical provides a good description of the time dependence of key gas phase species in α -pinene/NOx photooxidn. expts. carried out in the European Photo reactor (EUPHORE). Photochem. Ozone Creation Potentials (POCP) were calculated for the 106 non-aromatic non-methane VOC in MCM v3 for idealized conditions appropriate to north-west Europe, using a photochem. trajectory model. The POCP values provide a measure of the relative ozone forming abilities of the VOC. Where applicable, the values are compared with those calculated with previous versions of the MCM.

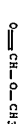
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 109-60-4, n-Propyl acetate 123-86-4, n-Butyl
 acetate 141-78-6, Ethyl acetate, reactions
 540-88-5, tert-Butyl acetate
 Rf: POL (pollutant); RCT (Reactant); OCCU (Occurrence); RACT
 (Reactant or reagent)
 (tropospheric degradation of non-aromatic volatile organic compds.)
 RN 78-79-5 HCAPLUS
 CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)



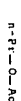
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 CN Acetic acid, methyl ester (CA INDEX NAME)



RN 107-31-3 HCAPLUS
 CN Formic acid, methyl ester (CA INDEX NAME)



RN 109-60-4 HCAPLUS
 CN Acetic acid, propyl ester (CA INDEX NAME)



CN 123-86-4 HCAPUS
 Acetic acid, butyl ester (CA INDEX NAME)
 n-Bu-O-Ac
 CN 141-78-6 HCAPUS
 Acetic acid ethyl ester (CA INDEX NAME)
 Et-O-Ac
 CN 540-88-5 HCAPUS
 Acetic acid, 1,1-dimethylethyl ester (CA INDEX NAME)
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 60-29-7, Diethyl ether, reactions 64-17-5, Ethanol, reactions
 64-18-5, Formic acid, reactions 64-19-7, Acetic acid, reactions
 67-56-1, Methanol, reactions 67-63-0, Propan-2-ol, reactions
 67-64-1, Propanone, reactions 67-66-3, Trichloromethane,
 reactions 71-23-6, Propan-1-ol, reactions 71-36-3, Butan-1-ol,
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 2-Methylpropan-2-ol, reactions 75-83-2, 2,2-Dimethylbutane
 75-85-4, 2-Methylbutan-2-ol 75-97-8, 3,3-Dimethylbutan-2-one
 78-78-4, 2-Methylbutane 78-79-5, 2-Methylbuta-1,3-diene,
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 reactions 79-09-4, Propanoic acid, reactions 79-20-9,
 Methyl acetate 79-29-8, 2,3-Dimethylbutane 80-56-8,
 α-Pinene 96-14-0, 3-Methylpentane 96-22-0, Pentan-3-one
 105-46-4, sec-Butyl acetate 106-97-8, Butane, reactions
 106-98-9, But-1-ene, reactions 106-99-0, Buta-1,3-diene,
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 Cyclohexanone, reactions 109-60-4, n-Propyl acetate
 109-66-0, Pentane, reactions 109-67-1, Pent-1-ene 109-86-4,
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 reactions 110-62-3, Pentanal 110-80-5, 2-Ethoxyethanol,
 reactions 110-82-7, Cyclohexane, reactions 111-65-9, Octane, reactions
 111-76-2, 2-Butoxyethanol 111-84-2, Nonane 112-40-3, Dodecane
 115-07-1, Propene, reactions 115-10-6, Dimethyl ether
 115-11-7, 2-Methylpropane, reactions 123-38-6, Propanal,
 reactions 123-42-2, 4-Hydroxy-4-methylpentan-2-one 123-51-3,

3-Methylbutan-1-ol 123-72-8, Butanal 123-66-4, n-Butyl
 acetate 124-18-5, Decane 127-18-4, Tetrachloroethene,
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 141-46-8 141-78-6, Ethyl acetate, reactions 142-82-5,
 Heptane, reactions 156-59-2, cis-1,2-Dichloroethene 156-60-5,
 trans-1,2-Dichloroethene 163-82-1, 2,2-Dimethylpropane
 513-35-9, 2-Methylbut-2-ene 540-88-5, tert-Butyl acetate
 563-45-1, 3-Methylbut-1-ene 563-46-2, 2-Methylbut-1-ene
 563-79-1, 2,3-Dimethylbut-2-ene 563-80-4, 3-Methylbutan-2-one
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 Hexan-3-one 590-18-1, cis-But-2-ene 591-76-4, 2-Methylhexane
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 11104-93-1, Nox, reactions 88181-75-3
 RI: POL (Pollutant); RCP (Reactant); OCCU (Occurrence); RACT
 (Reactant or reagent)
 (tropospheric degradation of non-aromatic volatile organic compounds)
 REFERENCE COUNT: 98
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 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

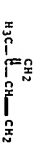
L74 ANSWER 27 OF 67 HCAPUS COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 2003.348333 HCAPUS Full-text
 DOCUMENT NUMBER: 139.89246
 TITLE:
 Speciation of volatile organic compound
 emissions for regional air quality modeling of
 particulate matter and ozone
 Makar, P. A.; Moran, M. D.; Scholtz, W. T.;
 Taylor, A.
 CORPORATE SOURCE:
 Modelling and Integration Division, Air
 Quality Research Branch, Meteorological
 Service of Canada, Toronto, ON, Can.
 SOURCE:
 Journal of Geophysical Research, [Atmospheres]
 (2003), 108(D2), ACH 2/1-ACH 2/51
 CODEN: JGRD23; ISSN: 0148-0227
 PUBLISHER:
 American Geophysical Union
 DOCUMENT TYPE:
 Journal
 LANGUAGE:
 English
 ED Entered STN: 08 May 2003
 AB
 A new classification scheme for speciation of organic compound emissions for use in air
 quality models is described. This scheme uses 81 organic compound classes to preserve
 net gas-phase reactivity and particulate matter (PM) formation potential. Chemical
 structure, vapor pressure, OH- reactivity, i.p./b.p., and solubility data were used to
 create the 81 compound classes. Volatile, semi-volatile, and non-volatile organic
 compounds are included. This classification scheme was used in conjunction with the
 Canadian Emissions Processing System (CEPS) to process 1990 gas- and particle-phase
 organic compound emissions data for summer and winter for a domain covering much of
 eastern North America. A simple post-processing model analyzed speciated organic
 emissions in terms of gas-phase reactivity and potential to form organic PM.
 Previously unresolved high-reactivity compounds which may significantly affect O3 formation
 included biogenic high-reactivity esters and internal C5-8 alkenes-alcs, and
 anthropogenic ethanol and propanol. Organic radical production associated with
 anthropogenic organic compound emissions may be 21 orders of magnitude more important
 than biogenic-associated production in northern USA and Canadian cities, and a factor
 of 3 more important in southern US cities. Previously unresolved organic compound
 classes, e.g., low vapor pressure polycyclic aromatic hydrocarbons (PAH), anthropogenic
 diacids, dialkyl phthalates, and high C number alkanes, may have a significant impact
 on organic particle formation. Primary organic particles (poorly characterized in
 national emissions databases) dominate total organic particle concns., followed by
 secondary formation and primary gas-particle partitioning. The effect of the assumed

Initial aerosol water concentration on subsequent thermodyn. calcs. suggested hydrophobic and hydrophilic comps. may form external mixts., and that sep. treatment for these groups may be required in future air quality model simulations. The post-processing model used overestimated organic particle formation relative to measurements, lacked the complexity of a regional air quality model, and was not intended as an alternative to the latter. However, post-processing model results do provide guidance for treating organic gases and particles in future air quality modeling work. Future air quality model simulations should attempt to speciate primary particulate organic comps. and include more detailed organic compound classes. Future emissions profile measurements should speculate gaseous high mol. mass organic comps. and primary orgs. emitted in particulate form (primary particle emissions are only available as a total particulate mass in currently available missions data).

IT

78-79-5, Isoprene, reactions 79-20-9, Methylnonadecanoate 80-62-6, Methylnonadecanoate 84-74-2, Dibutylphthalate 85-68-7, Butylbenzylphthalate 96-33-3, Methylnonadecanoate 105-37-3, 106-65-0, Dimethylbutanedioate 107-31-3, Methylformate 108-05-4, Vinyl acetate, reactions 108-21-4, Isopropyl acetate 109-60-4, n-Propylacetate 110-19-0, Isobutylacetate 111-19-9, Cellosolve acetate 111-82-0, Methyl dodecanoate 112-39-0, Methylpalmitate 112-61-8, Methyl stearate 120-61-6, Dimethylterephthalate 123-35-3, Myrcene 123-66-0, Ethylhexanoate 123-86-4, n-Butylacetate 124-10-7, Methyl myristate 131-11-3, Dimethylphthalate 136-60-7, Butylbenzoate 140-88-5, Ethylacetate 141-32-2, Butylacrylate 141-78-6, Ethylacetate, reactions 547-63-7, Methyl isobutyrate 627-93-0, Dimethylhexanedioate 119-40-0, Dimethyl pentanedioate RI: OCCU (Occurrence), BACT (Reactant or reagent) (Reactant); OCCU (Occurrence); BACT (Reactant or reagent) (volatile organic compound emission speciation for modeling regional air quality and particulate matter and ozone formation)

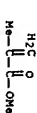
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RN 79-20-9 HCAPLUS
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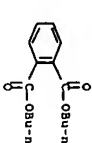


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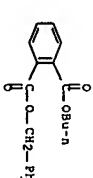


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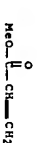
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RN 85-68-7 HCAPLUS
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CN 2-Propenoic acid, methyl ester (CA INDEX NAME)



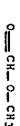
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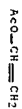
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CN Butenedioic acid, 1,4-dimethyl ester (CA INDEX NAME)



RN 107-31-3 HCAPLUS
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RN 108-05-4 HCAPLUS
CN Acetic acid ethenyl ester (CA INDEX NAME)



RN 108-21-4 HCAPLUS
CN Acetic acid, 1-methylethyl ester (CA INDEX NAME)



RN 109-60-4 HCAPLUS
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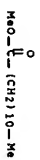
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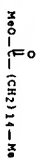
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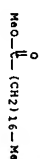
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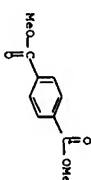
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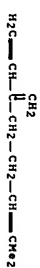
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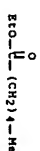
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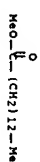
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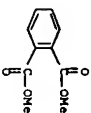
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CN Tetradecanoic acid, methyl ester (CA INDEX NAME)



RN 131-11-3 HCAPLUS



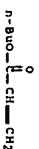
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RN 140-88-5 HCAPLUS
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RN 141-32-2 HCAPLUS
 CN 2-Propenoic acid, butyl ester (CA INDEX NAME)



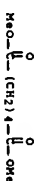
RN 141-78-6 HCAPLUS
 CN Acetic acid ethyl ester (CA INDEX NAME)



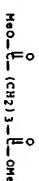
RN 547-63-7 HCAPLUS
 CN Propanoic acid, 2-methyl-, methyl ester (CA INDEX NAME)



RN 627-93-0 HCAPLUS
 CN Hexanedioic acid, 1,6-dimethyl ester (CA INDEX NAME)



RN 1119-40-0 HCAPLUS
 CN Pentanedioic acid, 1,5-dimethyl ester (CA INDEX NAME)



CC 59-2 (Air Pollution and Industrial Hygiene)

Section cross-reference(s): 53
 IT Aldehydes, reactions

Alkanes, reactions
 Alkenes, reactions
 Alkynes
 Amides, reactions
 Amines, reactions
 Carbonyl compounds (organic), reactions
 Epoxides
 Esters, reactions
 Ethers, reactions
 Hydrocarbons, reactions
 Ketones, reactions
 Naphtha
 Naphthenic acids, reactions
 Petroleum spirits
 Polyoxalkylenes, reactions
 Polysiloxanes, reactions
 Terpenes, reactions
 Thiols, reactions

Volatile organic compounds
 RL: OCU (Occurrence, unclassified); POL (Pollutant); RCT
 (Reactant); OCCU (Occurrence); RACT (Reactant or reagent)
 (volatile organic compound emission speciation for modeling regional
 air quality and particulate matter and ozone formation)

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 RL: OCU (Occurrence), unclassified); POL (Pollutant); RCT (Reactant); OCCU (Occurrence); ROCR (Reactant or reagent) (volatiles organic compound emission speciation for modeling regional air quality and particulate matter and ozone formation)
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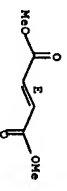
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12048-10-5, Tetrachlorobenzene 13269-32-8, trans-3-Hexene
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23354-52-3, Nonylphenol 25167-67-3, Butene 25265-71-8,
Dipropylene glycol 25321-09-9, Diisopropyl benzene 25321-22-6,
Dichlorobenzene
Rt: OCU (Occurrence, unclassified); POL (Pollutant); RCT
(Reactant); OCCU (Occurrence); RACT (Reactant or reagent)

(volatile organic compound emission speciation for modeling regional
air quality and particulate matter and ozone formation)
REFERENCE COUNT: 86 THERE ARE 86 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

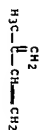
L74 ANSWER 28 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:881452 HCAPLUS FULL-TEXT
DOCUMENT NUMBER: 140:181474
TITLE: Product subclass 2: palladium-allyl complexes.
AUTHOR(S): Friesen, R. W.
CORPORATE SOURCE: Merck Frost Centre for Therapeutic Research,
Kirkland, PE, H9H 3J1, Can.
SOURCE: Science of Synthesis (2002), 1,
113-284
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
ED Entered STN: 21 Nov 2002
AB A review on preparation and application of palladium-allyl complexes.
IT 116-17-6, Triisopropyl phosphite 624-49-7,
Dimethyl fumarate
Rt: CAT (Catalyst and application); USES (Uses)
(preparation and application of palladium-allyl complexes)
RN 116-17-6 HCAPLUS
CN Phosphorous acid, tris(1-methylethyl) ester (CA INDEX NAME)

OP-1
1-PRO-1-OP-1

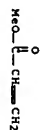
RN 624-49-7 HCAPLUS
CN 2-Butenedioic acid (2E)-, 1,4-dimethyl ester (CA INDEX NAME)
Double bond geometry as shown.



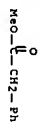
IT 78-79-5, 2-Methylbutadiene, reactions 96-33-3,
Methyl acrylate 101-61-7, Methyl phenylacetate
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acetate 108-59-8, Dimethyl malonate 115-95-7,
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141-12-8, Neryl acetate 141-97-9, Ethyl
acetoacetate 591-87-7, Allyl acetate 996-82-7,
Diethyl sodiomalonate 1191-16-8, 3-Methyl-2-butenyl
acetate 10544-63-5, Ethyl 2-butenolate 18424-76-5
Rt: RCT (Reactant); RACT (Reactant or reagent)
Rt: RCT (Reactant); RACT (Reactant or reagent)
RN 78-79-5 HCAPLUS
CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)



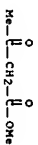
RN 96-33-3 HCAPLUS
CN 2-Propenoic acid, methyl ester (CA INDEX NAME)



RN 101-41-7 HCAPLUS
CN Benzenoacetic acid, methyl ester (CA INDEX NAME)

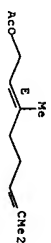


RN 105-45-3 HCAPLUS
CN Butanoic acid, 3-oxo-, methyl ester (CA INDEX NAME)

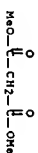


RN 105-87-3 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E) - (CA INDEX NAME)

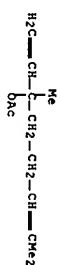
Double bond geometry as shown.



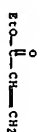
RN 108-59-8 HCAPLUS
CN Propanedioic acid, 1,3-dimethyl ester (CA INDEX NAME)



RN 115-95-7 HCAPLUS
CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)



RN 140-88-5 HCAPLUS
CN 2-Propenoic acid, ethyl ester (CA INDEX NAME)

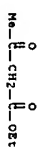


RN 141-12-8 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z) - (CA INDEX NAME)

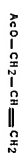
Double bond geometry as shown.



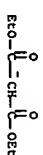
RN 141-97-9 HCAPLUS
CN Butanoic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



RN 591-87-7 HCAPLUS
CN Acetic acid, 2-propen-1-yl ester (CA INDEX NAME)



RN 996-82-7 HCAPLUS
CN Propanedioic acid, 1,3-diethyl ester, ion(1-), sodium (1:1) (CA INDEX NAME)



RN 1191-16-8 HCAPLUS
CN 2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)

AcO-CH₂-CH=CH₂

RN 10544-63-5 HCAPLUS
CN 2-Butenoic acid, ethyl ester (CA INDEX NAME)

EtO- $\overset{\text{O}}{\parallel}$ -CH=CH₂ Me

RN 18424-76-5 HCAPLUS
CN Propenedioic acid, dimethyl ester, ion(1-), sodium (1:1) (CA INDEX NAME)

MeO- $\overset{\text{O}}{\parallel}$ -CH- $\overset{\text{O}}{\parallel}$ -CH₂ OMe

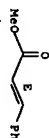
● Na⁺

IT 123-35-3P, β-Hyrcene
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)

H₂C=CH- $\overset{\text{CH}_2}{\parallel}$ -CH₂-CH₂-CH=CH₂ CH₃

IT 1754-62-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
RN 1754-62-7 HCAPLUS
CN 2-Propenoic acid, 3-phenyl-, methyl ester, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



CC 29-0 (Organometallic and Organometalloidal Compounds)
IT 95-45-4, Dimethylglyoxime 116-17-6, Trisopropyl Phosphite 546-89-4, Lithium acetate 624-49-7, Dimethyl fumarate 1067-52-3, Tributylmethoxystannane 2622-08-4,

Tri-*o*-tolyl phosphite 7447-41-8, Lithium chloride, uses 7688-25-7, Dppb 10377-51-2, Lithium iodide 12150-46-8, Dppf 14024-61-4, Palladium bis(acetoacetato) 14221-01-3
Tetrakis(triphenylphosphine)palladium 11830-50-1 28516-49-6, Tris(triphenylphosphine)palladium 31277-98-2, Bis[1,2-bis(diphenylphosphino)ethane]palladium 32305-98-9, (+)-BINAP 138517-61-0 141362-75-6 145964-33-6 18461-14-7 148461-16-9 154260-45-4 155184-93-3 156926-21-5 156975-04-1 159790-42-8 163591-42-2 166190-38-1 167171-03-1 188199-77-1 189210-88-6 190911-31-0 197918-40-4 210167-73-0 213269-97-7

RL: CAT (Catalyst use); USES (Uses)

IT (Preparation and application of palladium-allyl complexes)
57-83-0, Progesterone, reactions 58-22-0, Testosterone 62-53-3, Aniline, reactions 64-13-7, Acetic acid, reactions 65-85-0, Benzoic acid, reactions 67-56-1, Methanol, reactions 67-63-0, Isopropanol, reactions 70-55-3, Toluamide 74-85-1, Ethene, reactions 75-65-0, Tert-butyl alcohol, reactions 75-77-4, Trimethylsilyl chloride, reactions 78-59-1, Isophorone 78-79-5, 2-Methylbutadiene, reactions 78-88-6 78-94-4, Methyl vinyl ketone, reactions 79-24-3, Nitroethane 85-41-6, Pthalimide 90-39-1, (-)-Sparteine 96-33-3, Methyl acrylate 97-94-9, Triethylborane 98-86-2, Acetophenone, reactions 100-11-8, 4-Nitrobenzyl bromide 100-39-0, Benzyl bromide 100-44-7, Benzyl chloride, reactions 100-51-6, Benzyl alcohol, reactions 100-58-3, Phenylmagnesium bromide 101-41-7, Methyl phenylacetate 103-49-1, Dibenzylamine 103-54-8, Cinnamyl acetate 103-71-9, Phenyl isocyanate, reactions 104-82-5, 4-Methylbenzyl chloride 105-45-3, Methyl acetate 105-87-3, Geranyl acetate 106-99-0, Butadiene, reactions 107-05-1, Allyl chloride 107-13-1, Acrylonitrile, reactions 107-18-6, Allyl alcohol, reactions 107-40-4, 2,4,4'-Trimethyl-2-pentene 108-59-8, Dimethyl malonate 108-94-1, Cyclohexanone, reactions 108-95-2, Phenol, reactions 109-67-1, 1-Pentene 109-88-7, Diethylamine, reactions 110-83-8, Cyclohexene, reactions 111-71-7, Heptanal 112-31-2, Decanal 115-11-7, Isobutene, reactions 115-95-7, Linalyl acetate 122-39-4, Diphenylamine, reactions 123-54-6, Acetylacetone, reactions 124-13-0, Octanal 126-99-8, 2-Chlorobutadiene 140-29-4, Phenylacetoneitrile 140-88-5, Ethyl acrylate 141-12-8, Neryl acetate 141-97-9, Ethyl acetate 142-29-0, Cyclopentene 157-40-4, Spiropentene 463-49-0, Allene 497-53-8, 2-Methylmenorborane 503-60-6 513-81-5, 2,3-Dimethylbutadiene 532-31-0, Silver(I) benzoate 543-63-5, Butylmercuric chloride 554-61-0 563-47-3, Methylallyl chloride 563-52-0, 3-Chloro-1-butene 563-63-3, Silver(I) acetate 583-04-0, Allyl benzoate 590-18-1 591-49-1, 1-Methylcyclohexene 591-87-7, Allyl acetate 591-93-5, 1,4-Pentadiene 591-96-8, 1,3-Dimethylallene 591-97-9, 2-Butenyl chloride 592-41-6, 1-Hexene, reactions 592-57-4, 1,3-Cyclohexadiene 598-25-4, 1,1-Dimethylallene 601-57-0, Cholest-4-en-3-one 603-35-0, Triphenylphosphine, reactions 603-35-0D, Triphenylphosphine, reaction product from palladium dichloride dppc complex and DIBAL-H 609-02-9, Dimethyl methylenesuccinate 614-20-0 614-47-1, (E)-Benzylidenesuccinonone 615-99-6, Diallyl oxalate 618-41-7, Phenylsulfonic acid 623-43-8 627-20-3, (Z)-2-Pentene 628-08-0, 2-Butenyl acetate 629-20-9, Cyclooctatetraene 674-82-8, Diketene 689-06-5, 4-Methyl-3-hexen-2-one 693-86-7, Vinylcyclopropane 693-89-0, Trimethyl(vinyl)stannane 754-05-2, Trimethylvinylsilane 754-06-3, Trimethyl(vinyl)stannane 762-72-1, Allyltrimethylsilane 762-73-2, Allyltrimethylstannane 763-29-1, 2-Methyl-1-pentene 765-69-5, 2-Methyl-1,3-cyclopentadiene 820-57-5, Methylallyl formate 820-71-3, Methylallyl acetate 824-79-3, Sodium

p-toluenesulfonate 826-13-1, 827-69-0, 4-Phenylpent-3-en-2-one
827-87-2, 869-29-4, 873-55-2, Sodium phenylsulfinate
917-54-4D, Methylaluminum, reaction products with nickel
tetraacarbonyl 926-56-7, 4-Methyl-1,3-pentadiene 930-22-3,
vinylcyclohexane 930-30-3, 2-Cyclopenten-1-one 934-56-5,
Trimethylphenyltin 960-16-7, Tributylphenylstannane 993-07-7,
Trimethylphenyltin 996-82-7, Diethyl sodiomalonate
1000-66-8, 2,4-Dimethyl-1,3-pentadiene 1072-25-9, Heptylallene
1074-24-4, Potassium phthalimide 1167-33-5, 1184-88-9, Sodium
pivalate 1189-09-9, Methyl (E)-geranate 1191-16-8,
3-Methyl-2-butenyl acetate 1192-37-6, Methylcyclohexane
1196-73-2, 1205-42-1, 1424-22-2, 1450-14-2, Hexamethylallene
1458-99-7, 4-Chloropent-2-ene 1461-22-9, Tributylchlorostannane
1469-70-1, Allyl ethyl carbonate 1489-57-2, 2-Methyl-1,3-
Cyclohexadiene 1521-51-3, 3-Bromocyclohexene 1528-30-9,
Methylcyclopentane 1541-29-3, 1576-98-3, 1617-18-1, Ethyl
3-butenolate 1617-19-2, Ethyl 3-methyl-3-butenolate 1700-10-3,
1,3-Cyclooctadiene 1746-13-0, Allyl phenyl ether 1809-67-2,
1,896-62-4, 2001-45-8, Tetraphenylphosphonium chloride
2004-10-8, (E)-1,3-Pentadiene 2327-97-1, 1-Phenyl-1,2-pentadiene
2327-99-3, Phenylallene 2384-90-9, Butylallene 2442-10-6
2483-57-0, Methyl nitroacetate 2497-18-9, 2622-05-1,
Allylmagnesium chloride 2622-21-1, 1-Vinyl-1-cyclohexene
2637-34-5, 2-Sulfanylpiperidine 2684-62-0, Diazoacetone
2687-12-9, 3-Phenylallyl chloride 2749-96-4, p-Tolylallene
2783-10-0, 5-Methylhexa-1,3-diene 2923-17-3, Lithium
trifluoroacetate 2966-50-9, Silver(I) trifluoroacetate
3066-75-9, Allyl diethyl phosphate 3282-32-4, Phenyl diazomethyl
ketone 3618-12-0, Cyclohexene 3796-70-1, Geranylacetone
4054-38-0, 1,3-Cyclohexadiene 4074-22-0, 1,4-Dimethyl-1,4-
cyclohexadiene 4083-64-1, Tosyl isocyanate 4112-09-8
4157-02-2, 4358-59-2, 4372-94-5, 1,1-Dimethyl-2-ethoxy-2-
methylcyclopropane 4431-24-7, 1,2-Bis(diphenylamino) ethane
4483-16-9, 4-Methyl-3-heptene 4497-92-1, (+)-2-Carene
4663-22-3, 4720-83-6, 6-Oxabicyclo[3.2.1]oct-3-en-7-one
4683-61-2, (2)-3-Methoxy-19-norpregna-1,3,5(10),17(20)-tetraene
4883-67-4, 2-Nitrocyclohexanone 4894-61-5, (E)-1-Chlorobut-2-ene
4964-03-8, (E)-1-(Trimethylsilyl)prop-1-ene 5194-50-3,
(E,2)-Hexa-2,4-diene 5194-51-4, (E,E)-Hexa-2,4-diene
5389-87-7, Geranyl chloride 5395-20-0, Benzyl p-Tolyl sulfone
5459-93-0, 5489-14-5, Silver(I) propanoate 5674-01-1,
2-Methylallylmagnesium chloride 5732-13-8, 6088-88-6,
2-Butenylmagnesium chloride 6108-61-8, (Z,2)-Hexa-2,4-diene
6117-81-5, 2-Buten-1-ol 6142-73-0, Methylcyclopropane
6279-66-3, 6290-05-7, N,N-Bis(ethoxycarbonylmethyl)amine
6628-84-2, 6631-36-1, 6690-12-6, 6-Oxabicyclo[6.1.0]non-2-ene
6703-51-7, 7-Oxabicyclo[4.1.0]hept-2-ene 6737-11-7, 6790-37-0,
3,4-Epoxy-1-pentene 6790-38-1, Allyloxirane 6921-34-2,
Benzylmagnesium chloride 7129-41-1, 6-Oxabicyclo[3.1.0]hex-2-ene
7204-29-7, 7217-71-2, 7299-28-7, Tributyltin trifluoroacetate
7432-28-8, 7437-61-8, 7770-41-4, 10544-63-5, Ethyl
2-butenolate 12077-82-6, Bis(hex-3-en-2-yl)bis(hydroxymethyl)tin
12081-43-5, Bis(hydroxymethyl)tin(IV)bis(hydroxymethyl)tin
12103-44-1, 12138-25-5, 12211-09-1, 12463-39-3D, Nickel
tetraacetonate, reaction products and methylaluminum or
benzylmagnesium chloride 13466-78-9, 3-Carene 13505-10-7,
5-Methyl-4-hexen-3-one 14155-77-2, Allylmagnesium chloride
14219-90-0, Thallium acetate 14309-16-1, 14371-10-9
14483-67-1, tert-Butyl (trimethylsilyl) sulfide 14592-55-4,
Bis(acetonitrile)dichloropalladium 14750-79-9, 15022-08-9,
Diallyl carbonate 15525-45-8, Diallyl ether tetraethylenedipaladate
16510-49-9, 1,2,3-Triphenylcyclopropane 16732-86-8,
Al-Cholestene 16733-97-4, Cyclooctadienylaluminum
17094-21-2, 17351-28-9, 1,2-Dimethyl-1,4-cyclohexadiene
17442-12-7, 17447-60-8, 17851-97-7, 18025-87-4,
1,1,1-Trichloro-2,2,2-trimethylsilane 18424-76-5,

Diethyl sodiomalonate 18522-92-4, 18709-01-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(Preparation and application of palladium-allyl complexes)
100-02-7P, Benzaldehyde, preparation 123-35-3P,
β-Hyccene 930-68-7P, 2-Cyclohexen-1-one 1121-18-2P,
2-Methyl-2-cyclohexen-1-one 3112-87-6P, Allyl p-Tolyl sulfone
3724-55-8P, Methyl 3-butenolate 12081-18-4P, Bis(h-
chloro)(h3-2-methylallyl)palladium 12081-22-0P,
Bis(h3-2-butenyl)(h-chloro)palladium 14447-34-8P,
1639-57-4P, (E)-1-Phenyl-1,3-butadiene 20657-21-0P
2430-46-6P, 35998-93-7P, Tributyltin chloride 32007-86-6P, 3306-44-4P
33306-44-5P, 35989-97-2P, Tributyltin chloride 32007-86-6P, 3306-44-4P
53789-96-1P, 53789-97-2P, 53820-06-9P, 55803-94-8P
77773-11-6P, 77944-71-9P, 87567-12-2P
88076-44-2P, 91443-64-0P, 95177-49-4P, 95177-50-7P
100898-93-9P, 656837-12-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(Preparation and application of palladium-allyl complexes)
94-66-6P, 104-55-2P, Cinnamalddehyde 111-13-7P, Hexyl methyl
ketone 122-57-6P, 502-61-4P, (3E,6E)-α-Farnesene
601-11-6P, 5α-Cholest-2-en-1-one 601-55-8P,
5α-Cholest-1-en-3-one 818-98-6P, 877-94-1P,
5-Phenylpent-4-en-2-one 934-10-1P, 935-00-2P, 936-58-3P
936-67-4P, 2-Methylcyclohexanone 1002-35-3P, 1,3,7-Octatriene
1117-65-3P, 1120-73-6P, 2-Methylcyclopent-2-en-1-one 1123-34-8P
1205-84-1P, (E)-Ethyl 4-phenyl-3-butenolate 1208-44-2P
1271-03-0P, (h3-Allyl)(h5-cyclopentadienyl)palladium
1489-50-5P, 2-Methylcyclopent-1-en-1-one 1536-88-7P
1674-08-4P, trans-Biocrocinol 1754-62-7P, 2436-90-0P
2482-22-0P, 2609-23-9P, 3045-76-9P, 3045-98-5P, 3338-55-4P
3391-26-7P, 3491-27-8P, 3664-60-6P, 7-Octen-2-one
3710-30-3P, 1,7-Octadiene 3779-61-1P, 4063-60-8P, 4096-34-8P,
3-Cyclohexen-1-one 4187-81-9P, 4734-90-1P, 3-Cycloocten-1-one
5428-09-1P, 5558-87-2P, 5629-57-2P, 5666-17-1P, 6052-63-7P
6610-21-5P, 6-Methyl-2-cyclohexen-1-one 6728-26-3P,
(E)-Hex-2-enal 7065-05-6P, 7688-51-9P, 10066-38-9P
10281-55-7P, 10281-56-8P, 10428-96-3P, 10491-63-1P
10500-10-1P, 10500-11-5P, 10521-97-8P, 5-Phenylpent-3-en-2-one
12012-87-2P, Bis(h-chloro)(h3-2-chloroallyl)palladium
12080-98-7P, 12084-71-8P, Bis(h-aceto)bis(h3-
allyl)dipalladium 12090-04-9P, 12090-09-4P, 12090-69-6P
12097-84-6P, (h3-Allyl)chloro(triphenylphosphine)palladium
12099-33-1P, 12111-41-0P, 12129-99-6P, 12131-44-1P,
Bis(h-chloro)(h3-1-phenylallyl)palladium 12145-53-8P
12154-16-4P, 12156-09-1P, 12182-26-2P, 12240-87-8P,
Bis(h3-allyl)palladium 12245-05-5P, 12245-22-6P
12245-27-1P, 12245-28-2P, 12245-51-1P, 12245-52-5P
12245-53-3P, 12245-70-4P, 12246-02-5P, 12281-94-6P
12288-41-4P, 12301-06-3P, 12302-55-4P, 12308-56-4P
12309-85-2P, 12395-90-4P, 13891-96-8P, 1-Undecen-1-ol
14320-37-7P, Cyclopent-3-en-1-one 14543-49-8P, 14815-73-7P
14815-74-8P, 15232-96-9P, 15874-80-3P, 16178-87-3P
16215-11-5P, 16424-35-4P, 16515-65-8P, 16717-84-3P
16818-61-4P, 18355-02-4P, 18355-70-9P, 18956-05-3P
19043-46-0P, 19752-23-9P, 20068-10-4P, (E)-4-Phenyl-1,3-
butenediol 20202-62-4P, 20230-16-4P, 20337-59-9P
20461-31-8P, 21473-05-2P, 21488-83-5P, (Z)-1-Phenyl-3,7-
diethyl-2,6-diene 21677-96-3P, 21860-49-1P, 25564-22-1P
25893-52-3P, Methyl 3-methyl-3-butenolate 26450-24-8P
26482-12-3P, 26561-31-9P, 26561-32-0P, 26828-28-8P
27829-72-3P, 28973-98-0P, 29085-37-8P, 29330-76-5P
29330-77-6P, 29330-85-6P, 29330-86-7P, 30463-55-9P
31666-74-7P, 31666-77-0P, 31985-02-1P, 32064-72-5P,

2-Nonen-4-one 3267-81-9P 32715-98-3P 32732-73-3P
 32876-08-7P 32915-63-2P 32965-48-3P 33155-42-9P
 33379-48-5P 35284-32-3P 35396-78-2P 36321-95-6P
 36351-77-6P 36510-65-3P 36572-87-9P 36971-14-9P,
 1-Decen-4-ol 37464-41-8P 37575-80-7P 38282-07-4P
 38342-40-4P 38342-41-5P 40637-56-7P 40695-04-3P
 41348-25-8P 41449-89-2P 41557-81-7P 41562-41-8P
 41656-05-7P 42762-56-1P 42998-16-3P 49676-93-5P
 50404-95-0P 50487-71-3P 50507-72-7P 50994-84-8P
 51042-92-3P 51106-45-7P 51106-47-9P 51106-50-4P
 51106-51-5P 51106-53-7P 51106-54-8P 51729-84-1P
 52389-75-0P 52922-10-8P 52922-19-7P 53254-60-7P
 53265-48-8P 54162-19-5P 54340-71-5P 54829-97-9P
 54829-98-0P 54897-36-8P 54962-87-7P 55053-65-1P
 5512-78-7P, 1-Eicosen-3-one 55454-04-1P 55613-91-5P
 55684-63-4P 55903-11-2P 56084-53-8P 56505-44-3P
 57321-30-3P 57981-18-7P 58355-66-1P 58482-97-6P
 58527-00-7P 59053-07-1P 60038-55-3P 60410-18-6P
 60729-61-5P 60729-63-7P 61113-02-8P 61113-03-9P
 61113-04-0P 61128-77-6P 61168-10-3P, 1-Nonen-4-one
 61187-40-4P 61305-24-6P 61342-31-2P 61761-21-5P
 61929-77-9P 62015-29-6P 62075-33-6P 62713-56-8P
 63138-98-7P 63812-05-5P 63817-37-8P 64841-68-5P
 65178-51-0P 65280-46-8P 65337-70-4P 65629-73-4P
 67099-84-7P 67393-58-2P 67450-36-6P 67463-14-3P
 67679-06-5P 67866-38-8P 67738-90-3P 67883-63-0P
 68276-71-1P 68284-22-0P 68340-12-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (Preparation and application of palladium-allyl complexes)
 THERE ARE 379 CITED REFERENCES AVAILABLE
 579 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L74 ANSWER 29 OF 67 HCAPLUS COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 2003:169267 HCAPLUS Full-text
 DOCUMENT NUMBER: 139:353491
 TITLE: UK specified VOC emission inventories
 AUTHOR(S): Passant, N.; Woodfield, M.; Hayman, G.
 CORPORATE SOURCE: AEA Technology, National Environmental
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 SOURCE: Troposphere and Chemical Transformation in the
 Troposphere, Proceedings of EUROTRAC
 Symposium, 7th, Garmisch-Partenkirchen,
 Germany, Mar. 11-15, 2002 (2002),
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 CODEN: 69DQJ7; ISBN: 3-8236-1385-5
 CONFERENCE: Conference (computer optical disk)
 DOCUMENT TYPE: English
 LANGUAGE: English
 ED Entered STN: 06 Mar 2003
 AB Volatile organic compds. (VOC), together with NOx lead to formation of ground-level O3.
 Over the past 10 yr, the UK has prepared specified emission inventories of VOC to
 support the development of policies to control ground-level O3 formation. Preparation
 of a specified VOC emission inventory is described and issues raised in its preparation
 and its subsequent validation against ambient hydrocarbon measurements are discussed.
 IT 78-73-5, Isoprene, reactions 79-20-9,
 Methylacetate 123-66-4, Butyl acetate 141-78-6
 , Ethyl acetate, reactions
 RL: OCU (Occurrence, unclassified); POL (Pollutant); RCT
 (Reactant); OCUC (Occurrence); RACT (Reactant or reagent)
 (ground-level ozone formation in relation to specified volatile
 organic compound emission inventory in UK)
 RN 78-79-5 HCAPLUS
 CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)

CH3-C(=O)-CH=CH-CH3
 RN 79-20-9 HCAPLUS
 CN Acetic acid, methyl ester (CA INDEX NAME)

CH3-C(=O)-CH3
 RN 123-86-4 HCAPLUS
 CN Acetic acid, butyl ester (CA INDEX NAME)

n-Bu-O-Ac
 RN 141-78-6 HCAPLUS
 CN Acetic acid ethyl ester (CA INDEX NAME)

Et-O-Ac

CC 59-2 (Air Pollution and Industrial Hygiene)
 IC Alcohols, reactions
 Aldehydes, reactions
 Alkanes, reactions
 Alkenes, reactions
 Alkynes
 Aromatic hydrocarbons, reactions
 Esters, reactions
 Hydrocarbons, reactions
 Ketones, reactions
 Volatile organic compounds
 RL: OCUC (Occurrence, unclassified); POL (Pollutant); RCT
 (Reactant); OCUC (Occurrence); RACT (Reactant or reagent)
 (ground-level ozone formation in relation to specified volatile
 organic compound emission inventory in UK)
 IT 64-11-5, Ethanol, reactions 67-56-1, Methanol, reactions
 67-61-0, 2-Propanol, reactions 67-64-1, Acetone, reactions
 68-12-2, Dimethylformamide, reactions 71-36-3, 1-Butanol,
 reactions 71-43-2, Benzene, reactions 74-84-0, Ethane,
 reactions 74-85-1, Ethylene, reactions 74-86-3, Chloromethane,
 reactions 74-86-6, Propene, reactions 75-00-3, Chloroethane,
 reactions 75-09-2, Dichloroethane,
 reactions 75-28-5, Isobutane 75-35-4, 1,1-Dichloroethene,
 reactions 78-78-4, Isopentane 78-79-5, Isoprene,
 reactions 78-83-1, 2-Methyl-1-propanol, reactions 78-93-3,
 2-Butanone, reactions 79-01-6, Trichloroethene, reactions
 79-10-7, Acrylic acid, reactions 79-20-9, Methylacetate
 95-47-6, o-Xylene, reactions 96-14-0, 3-Methylpentane
 100-41-4, Ethylbenzene, reactions 106-42-3, p-Xylene, reactions
 106-97-8, Butene, reactions 106-98-9, 1-Butene, reactions

106-99-0, 1,3-Butadiene, reactions 107-06-2, 1,2-Dichloroethane, reactions 107-83-5, 2-Methylpentane 108-10-1, 4-Methyl-2-pentanone 108-38-3, m-Xylene, reactions 108-65-6, 1-Methoxy-2-propylacetate 108-88-3, Toluene, reactions 109-66-0, Benzene, reactions 110-54-3, Hexane, reactions 111-76-2, 2-Butoxyethanol 123-86-4, Butyl acetate reactions 115-10-6, Dimethylether 123-86-4, Butyl acetate reactions 141-78-6, Ethyl acetate, reactions 142-82-5, n-Heptane, reactions 590-18-1, cis-2-Butene 624-64-6, trans-2-Butene 627-20-3, cis-2-Pentene 646-04-8, trans-2-Pentene 7397-62-8, Butyl glycolate 7446-09-5, Sulfur dioxide, reactions 7664-41-7, Ammonia, reactions 1104-93-1, Nitrogen oxide, reactions

RL: OCCU (Occurrence, unclassified); POL (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or reagent) (ground-level ozone formation in relation to specified volatile organic compound emission inventory in UK)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 30 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:808833 HCAPLUS Full-Text
 DOCUMENT NUMBER: 136:155317
 TITLE: Characterization of the reactivities of volatile organic compounds using a master chemical mechanism
 AUTHOR(S): Derwent, Richard G.; Jenkin, Michael E.; Saunders, Sandra M.; Pilling, Michael J.
 CORPORATE SOURCE: Climate Research Division, Meteorological Office, Bracknell, UK
 SOURCE: Journal of the Air & Waste Management Association (2001), 51(5), 699-707
 CODEN: JAWAFC; ISSN: 1096-2247
 PUBLISHER: Air & Waste Management Association
 LANGUAGE: English
 ED Entered STN: 07 Nov 2001

AB A comprehensive description of the O₃-forming potential of 101 organic compounds developed under North American urban averaged conditions using a detailed master chemical mechanism and a simple air parcel trajectory model. This chemical mechanism describes reactions of 3603 chemical species occurring in >10,500 chemical reactions. An index value, calculated for each organic compound, describes the increment in O₃ concentration observed downwind from an urban area following emission of a fixed increment in the mass emission of each organic compound. These indexes, termed photochem. O₃ creation potentials (POCP), were expressed on a scale relative to ethylene (ethene) = 100; a reactivity scale was generated for alkenes, alkenes, and oxygenated and halogenated organic compounds. A high degree of correlation (R² = 0.9) was observed between these POCP values and the most widely accepted urban reactivity scale. While reactivity of most of the 86 organic compounds compared fell within a consistent range, significant discrepancies were noted for only 5 compounds. Single- or multi-day conditions appeared important in establishing quant. reactivity scales for less reactive organic compounds.

IT 78-79-5, Isoprene, reactions 79-20-9, Methyl acetate 107-31-3, Methyl formate 108-21-4, Isopropylacetate 109-60-4, n-Propylacetate 123-86-4, n-Butylacetate 141-78-6, Ethyl acetate, reactions 540-88-5, tert-Butylacetate
 RL: POL (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or reagent)
 (master chemical mechanism model to characterize atmospheric reactivity of volatile organic compounds, and their ozone formation potential under North American urban average conditions)
 RN 78-79-5 HCAPLUS
 CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)

CC(=O)O
 RN 79-20-9 HCAPLUS
 CN Acetic acid, methyl ester (CA INDEX NAME)

CC(=O)OCC
 RN 107-31-3 HCAPLUS
 CN Formic acid, methyl ester (CA INDEX NAME)

CC(=O)OCC
 RN 108-21-4 HCAPLUS
 CN Acetic acid, 1-methylethyl ester (CA INDEX NAME)

CC(=O)OCC
 RN 109-60-4 HCAPLUS
 CN Acetic acid, propyl ester (CA INDEX NAME)

CC(=O)OCC
 RN 123-86-4 HCAPLUS
 CN Acetic acid, butyl ester (CA INDEX NAME)

CC(=O)OCC
 RN 141-78-6 HCAPLUS
 CN Acetic acid ethyl ester (CA INDEX NAME)

CC(=O)OCC
 RN 540-88-5 HCAPLUS
 CN Acetic acid, 1,1-dimethylethyl ester (CA INDEX NAME)

CC

Section cross-reference(s): 53

59-2 (Air Pollution and Industrial Hygiene)
 50-00-0, Formaldehyde, reactions 57-55-6, Propylene glycol, reactions 60-29-7, Diethylether, reactions 64-17-5, Ethyl alcohol, reactions 64-18-6, Formic acid, reactions 64-19-7, Acetic acid, reactions 67-56-1, Methyl alcohol, reactions 67-66-3, Chloroform, reactions 71-23-8, n-Propanol, reactions 71-36-3, Chloroform, reactions 71-55-6, Methyl chloroform 74-84-0, Ethane, reactions 74-85-1, Ethylene, reactions 74-87-3, Methyl chloride, reactions 74-98-6, Propane, reactions 75-07-0, Acetaldehyde, reactions 75-09-2, Methylene chloride, reactions 75-28-5, Isobutane 75-65-0, tert-butanol, reactions 75-83-2, 2,2-Dimethylbutane 75-85-4, 2-Methyl-2-butanol 75-97-8, Methyl-tert-butylketone 78-78-4, Isopentane 78-79-5, Isoprene, reactions 78-83-1, Isobutanol, reactions 78-84-2, Isobutylaldehyde 78-92-2, sec-Butanol 78-93-3, Methylcyclohexane, reactions 79-01-6, Trichloroethylene, reactions 79-09-4, Propionic acid, reactions 79-20-9, Methyl acetate 79-29-8, 2,3-Dimethylbutane 80-56-8, a-Pinene 96-14-0, 3-Methylpentane 96-22-0, Diethylketone 105-46-4, sec-Butylacetate 106-97-8, n-Butane, reactions 106-98-9, But-1-ene, reactions 106-99-0, 1,3-Butadiene, reactions 107-21-1, Ethylene glycol, reactions 107-31-3, Methyl formate 107-83-5, 2-Methylpentane 107-87-9, Methylpropylketone 107-98-2, 1-Methoxy-2-propanol 108-10-1, Methylisobutylketone 108-20-3, Diisopropylether 108-21-4, Isopropylacetate 108-93-0, Cyclohexanol, reactions 108-94-1, Cyclohexanone, reactions 109-60-4, n-Propylacetate 109-66-0, n-Pentane, reactions 109-67-1, Pent-1-ene 109-86-4, 2-Methoxyethanol 110-55-3, n-Hexane, reactions 110-62-9, Valeraldehyde 110-80-5, 2-Ethoxyethanol 110-82-7, Cyclohexane, reactions 111-65-9, n-Octane, reactions 111-76-2, 2-Butoxyethanol 111-84-2, n-Nonane 112-40-3, n-Dodecane 115-07-1, Propylene, reactions 115-10-6, Dimethylether 123-38-6, Propionaldehyde, reactions 123-42-2, Diacetone alcohol 123-51-3, 3-Methyl-1-butanol 123-72-8, Butylaldehyde 123-86-4, n-Butylacetate 124-18-5, n-Decane 127-18-4, Tetrachloroethylene, reactions 137-32-6, 2-Methyl-1-butanol 141-78-6, Ethyl acetate, reactions 142-82-5, n-Heptane, reactions 156-59-2, cis-Dichloroethylene 156-60-5, 463-82-1, Neopentane 513-35-9, 2-Methylbut-2-ene 540-88-5, tert-Butylacetate 563-45-1, 3-Methylbut-1-ene 563-46-2, 2-Methylbut-1-ene 563-80-4, Methylisopropylketone 584-02-1, 3-Pentanol 589-34-4, 3-Methylhexane 589-38-8, Hexan-3-one 590-18-1, cis-But-2-ene 591-76-4, 2-Methylhexane 591-78-6, Hexan-2-one 592-41-6, Hex-1-ene, reactions 598-75-4, 3-Methyl-2-butanol 624-64-6, trans-But-2-ene 627-20-3, cis-Pent-2-ene 637-92-3, Ethyl-tert-butylether 646-04-8, trans-Pent-2-ene 1120-21-4, n-Undecane 1634-04-4, Methyl-tert-butylether 2278-22-0, Peroxyacetyl nitrate 4050-45-7, trans-Hex-2-ene 5131-66-8, 1-Butoxy-2-propanol 7688-21-3, cis-Hex-2-ene 7697-37-2, Nitric acid, reactions 10102-43-9, Nitric oxide, reactions 10102-44-0, Nitrogen dioxide, reactions 11104-93-1, Nitrogen oxide, reactions 25167-67-3, Butylene
 RL: POL (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or reagent)
 (master chemical mechanism model to characterize atmospheric reactivity of volatile organic compounds, and their ozone formation potential)

under North American urban average conditions)
 REFERENCE COURT: 44
 THERE ARE 44 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L74 ANSWER 31 OF 67 HCAPUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:14306 HCAPUS FULL-TEXT
 DOCUMENT NUMBER: 134:270429
 TITLE: Prediction of flammability of gases by using F-number analysis
 AUTHOR(S): Kondo, S.; Umano, Y.; Tokunashi, K.; Takahashi, A.; Tanaka, K.
 CORPORATE SOURCE: Research Institute of Innovative Technology for the Earth, National Institute of Materials and Chemical Research, Tsukuba, Ibaraki, 305-0046, Japan
 SOURCE: Journal of Hazardous Materials (2001 1, 82(2), 113-128
 CODEN: JHMA09; ISSN: 0304-3894
 Elsevier Science B.V.
 English
 PUBLISHER: Journal
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 28 Feb 2001

AB A method of predicting flammability limits uses a flammability index called F-number. For this purpose, an empirical expression of F-number was derived to account for the flammability characteristics of various organic substances. The anal. was done by fitting to the observed values of F-number for a wide variety of organic gases and vapors. F-number is an excellent tool to analyze the flammability characteristics of various substances. Upper and lower flammability limits can be derived from F-number together with the stoichiometric concentration collected for the effect of selective diffusion.

IT 78-79-5, Isoprene, reactions 79-20-9, Methylacetate 80-62-6, Methylmethacrylate 96-33-3, Methyl acrylate 96-34-4, Methyl chloroacetate 105-37-3, Ethylpropionate 107-31-3, Methyl formate 108-05-4, Vinyl acetate, reactions 108-21-4, Iso propylacetate 109-60-4, Propylacetate 109-94-4, Ethyl formate 110-19-0, Isobutyl acetate 110-49-6, Methyl cellosolve acetate 111-55-7, Glycol diacetate 123-86-4, Butyl acetate 123-82-2, Isobutyl acetate 140-88-5, Ethyl acrylate 141-32-2, Butylacrylate 141-78-6, Ethyl acetate, reactions 141-97-9, Ethyl acetoacetate 554-12-1, Methylpropionate 592-84-7, Butylformate 628-63-7, Amyl acetate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Prediction of flammability of gases by using F-number anal.)
 RN 78-79-5 HCAPUS
 CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)

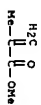
CH₃
 $\text{H}_3\text{C}-\text{CH}=\text{CH}_2$
 CH₂

H₃C- $\overset{\text{O}}{\underset{\text{O}}{\text{C}}}$ -CH₃

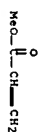
RN 79-20-9 HCAPUS
 CN Acetic acid, methyl ester (CA INDEX NAME)

SN 10/564307 Page 79 of 139 STIC STN SEARCH 5/17/2007

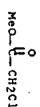
RN 80-62-6 HCAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester (CA INDEX NAME)



RN 96-33-3 HCAPLUS
CN 2-Propenoic acid, methyl ester (CA INDEX NAME)



RN 96-34-4 HCAPLUS
CN Acetic acid, 2-chloro-, methyl ester (CA INDEX NAME)



RN 105-37-3 HCAPLUS
CN Propanoic acid, ethyl ester (CA INDEX NAME)



RN 107-31-3 HCAPLUS
CN Formic acid, methyl ester (CA INDEX NAME)



RN 108-05-4 HCAPLUS
CN Acetic acid ethenyl ester (CA INDEX NAME)



RN 108-21-4 HCAPLUS
CN Acetic acid, 1-methylethyl ester (CA INDEX NAME)

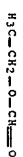
SN 10/564307 Page 80 of 139 STIC STN SEARCH 5/17/2007



RN 109-60-4 HCAPLUS
CN Acetic acid, propyl ester (CA INDEX NAME)



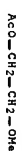
RN 109-94-4 HCAPLUS
CN Formic acid, ethyl ester (CA INDEX NAME)



RN 110-19-0 HCAPLUS
CN Acetic acid, 2-methylpropyl ester (CA INDEX NAME)



RN 110-48-6 HCAPLUS
CN Ethanol, 2-methoxy-, 1-acetate (CA INDEX NAME)



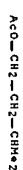
RN 111-58-7 HCAPLUS
CN 1,2-Ethanedithiol, 1,2-diacetate (CA INDEX NAME)



RN 123-86-4 HCAPLUS
CN Acetic acid, butyl ester (CA INDEX NAME)



RN 123-92-2 HCAPLUS
CN 1-Butanol, 3-methyl-, 1-acetate (CA INDEX NAME)



RN	140-08-5	HCAPLUS
CN	2-Propenoic acid, ethyl ester	(CA INDEX NAME)
	$\text{EtO}-\overset{\text{O}}{\underset{\text{CH}_2}{\text{CH}}}=\text{CH}_2$	
RN	141-32-2	HCAPLUS
CN	2-Propenoic acid, butyl ester	(CA INDEX NAME)
	$\text{n-BuO}-\overset{\text{O}}{\underset{\text{CH}_2}{\text{CH}}}=\text{CH}_2$	
RN	141-78-6	HCAPLUS
CN	Acetic acid ethyl ester	(CA INDEX NAME)
	$\text{Et}-\text{O}-\overset{\text{O}}{\text{C}}-\text{CH}_2-\text{CH}_2-\text{O}-\text{Ac}$	
RN	141-97-9	HCAPLUS
CN	Butanoic acid, 3-oxo-, ethyl ester	(CA INDEX NAME)
	$\text{Me}-\overset{\text{O}}{\underset{\text{CH}_2}{\text{C}}}-\overset{\text{O}}{\text{C}}-\text{CH}_2-\text{OEt}$	
RN	554-12-1	HCAPLUS
CN	Propanoic acid, methyl ester	(CA INDEX NAME)
	$\text{MeO}-\overset{\text{O}}{\text{C}}-\text{CH}_2-\text{CH}_2-\text{OEt}$	
RN	592-84-7	HCAPLUS
CN	Formic acid, butyl ester	(CA INDEX NAME)
	$\text{n-Bu}-\text{O}-\text{CHO}$	
RN	628-63-7	HCAPLUS
CN	Acetic acid, pentyl ester	(CA INDEX NAME)

CC	59-5 (Air Pollution and Industrial Hygiene)
IT	57-55-6, Propylene glycol, reactions 60-29-7, Ethylether, reactions 62-53-3, Aniline, reactions 64-17-5, Ethyl alcohol, reactions 64-19-7, Acetic acid, reactions 67-56-1, Methyl alcohol, reactions 67-63-0, Iso propyl alcohol, reactions 67-64-1, Acetone, reactions 71-23-8, Propyl alcohol, reactions 71-36-3, Butyl alcohol, reactions 71-41-0, Amyl alcohol, reactions 71-43-2, Benzole, reactions 71-55-6, 1,1,1-Trichloroethane 74-82-8, Methane, reactions 74-83-9, Methyl bromide, reactions 74-84-0, Ethane, reactions 74-85-1, Ethylene, reactions 74-86-2, Acetylene, reactions 74-87-3, Methyl chloride, reactions 74-89-5, Methylamine, reactions 74-96-4, Ethyl bromide 74-98-6, Propane, reactions 75-00-3, Ethyl chloride 75-01-4, Vinylchloride, reactions 75-02-5, Vinylfluoride 75-04-7, Ethylamine, reactions 75-05-8, Acetonitrile, reactions 75-07-0, Acetaldehyde, reactions 75-09-2, Methylene chloride, reactions 75-10-5, Ethylene oxide, reactions 75-19-4, Cyclopropane 75-21-8, Ethylene oxide, reactions 75-28-5, Iso butane 75-29-6, Iso propyl chloride 75-35-4, Vinylidene chloride, reactions 75-37-6, 1,1-Difluoroethane 75-38-7, Vinylidene fluoride 75-56-9, Propylene oxide, reactions 75-64-9, Tert butylamine, reactions 75-65-0, Tert butyl alcohol, reactions 75-68-3, 1-Chloro-1,1-difluoroethane 75-83-2, 2,2-Dimethylbutane 75-85-4, 2-Methyl-2-butanol 75-86-5, Acetone cyanohydrin 78-78-4, Isopentane 78-79-5, Isoprene, reactions 78-83-1, Iso butyl alcohol, reactions 78-84-2 78-87-5, Propylene dichloride 78-88-6, 2,3-Dichloropropene 78-92-2, 2-Butanol 78-94-4, Methyl vinyl ketone, reactions 79-01-6, Trichloroethylene, reactions 79-09-4, Propionic acid, reactions 79-10-7, Acrylic acid, reactions 79-20-9, Methylacetate 79-29-8, 2,3-Dimethylbutane 79-31-2, Iso butyric acid 79-46-9, 2-Nitropropane 80-62-6, Methylmethacrylate 85-44-9, Phthalic anhydride 91-20-3, Naphthalene, reactions 92-52-4, Biphenyl, reactions 95-47-6, o-Xylene, reactions 95-50-1, o-Dichlorobenzene 96-14-0, 3-Methylpentane 96-32-3, Methyl acrylate 96-34-4, Methyl chloroacetate 96-37-7, Methylcyclopentane 97-72-3, Isobutyric anhydride 97-96-1 97-99-4, Tetrahydrofurfuryl alcohol 98-00-0, Furfuryl alcohol 98-01-1, Furfural, reactions 98-06-6, Tert Butylbenzene 98-82-8, Cumene 100-41-4, Ethylbenzene, reactions 100-42-5, Styrene, reactions 103-09-3, 2-Ethylhexylacetate 103-65-1, Propylbenzene 104-51-8, Butylbenzene 104-76-7, 2-Ethylhexanol 105-05-5, p-Diethylbenzene 105-30-6 105-37-3, Ethylpropionate 105-46-4, Sec Butyl Acetate 105-57-7, Acetal 106-31-0, Butyric anhydride 106-42-3, p-Xylene, reactions 106-86-7, 1,2-Butylene oxide 106-89-8, Epichlorohydrin, reactions 106-95-6, Allyl bromide, reactions 106-97-8, Butane, reactions 106-98-9, 1-Butene, reactions 106-99-0, 1,3-Butadiene, reactions 107-02-8, Acrolein, reactions 107-05-1, Allyl chloride 107-06-2, Ethylene chloride, reactions 107-07-3, 2-Chloroethanol, reactions 107-10-8, Propylamine, reactions 107-11-9, Allylamine 107-13-1, Acrylonitrile, reactions 107-15-3, Ethylenediamine, reactions 107-18-6, Allyl alcohol, reactions 107-31-3, Methyl formate 107-83-5, Isohexane 107-87-9, Methylpropylketone 107-92-6, Butyric acid, reactions 108-05-4, Vinyl acetate, reactions 108-10-1, Methyl isobutyl ketone 108-11-2, Methyl isobutylcarbinol 108-18-9, Di-iso-propylamine 108-20-3, Isopropyl ether 108-21-4, Iso propylacetate 108-24-7, Acetic anhydride 108-31-6, Maleic anhydride, reactions 108-38-3, reactions

108-83-8, Di-isobutylketone 108-84-9, 108-87-2, 108-88-3, Di-isobutylketone 108-88-3, Toluol, reactions 108-90-7, Chlorobenzene, reactions 108-94-1, Cyclohexanone, reactions 109-66-4, Propylacetate 109-65-9, Butyl bromide 109-69-3, Butyl chloride 109-73-9, Butylamine, reactions 109-87-5, Vinyl ethyl ether 109-93-3, Divinyl ether 109-94-4, Ethyl formate 109-99-9, Tetrahydrofuran, reactions 110-00-9, Furan 110-12-3, Methylisobutylketone 110-19-0, Isobutyl acetate 110-43-0, Methylamylketone 110-49-6, Methyl cellosolve acetate 110-54-3, Hexane, reactions 110-58-7, Amylamine 110-82-7, Cyclohexane, reactions 110-88-3, Trioxane, reactions 11-43-3, Morpholine, reactions 11-40-0, Diethylene triamine 11-65-9, Octane, reactions 11-84-2, Nonane 11-27-6, Triethylene glycol 115-07-1, Propylene, reactions 115-10-6, Tetraethene 115-11-7, 2-Methylpropene, reactions 116-14-3, Tetrafluoroethylene, reactions 123-05-7, 2-Ethylhexanal 123-51-3, Isoamyl alcohol 123-82-6, Propionic anhydride 123-72-8, Butyl aldehyde 123-86-4, Butyl acetate 123-91-1, p-Dioxane, reactions 123-92-2, Isoamyl acetate 124-18-5, Decane 124-40-3, Dimethylamine, reactions 126-98-7, Methylacrylonitrile 126-99-8, 2-Chloro-1,3-butadiene 135-98-8, Sec Butylbenzene 140-88-5, Ethyl acrylate 141-32-2, Butylacrylate 141-78-6, Ethyl acetate, reactions 141-79-7, Mesityl oxide 141-97-9, Ethyl acetate 142-82-5, Heptane, reactions 142-96-1, Dibutyl ether 149-57-5, 2-Ethylhexanoic acid 151-56-4, Ethylamine, reactions 291-64-5, Cyclohexane 430-66-0, 1,1,2-Trifluoroethane 463-82-1, 2,2-Dimethylpropene 513-36-0, Iso butyl chloride 538-93-2, Isobutylbenzene 540-67-0, Propyl chloride 540-59-0, 1,2-Dichloroethane 540-67-0, Methyl ethyl ether 542-55-2, Iso butylformate 542-75-6, 1,3-Dichloropropene 554-12-1, Methylpropionate 563-45-1, 3-Methyl-1-butene 563-47-3, Methyllyl chloride 564-02-3, 2,2,3-Trimethylpentane 565-59-3, 2,3-Dimethylpentane 584-02-1, 3-Pentanol 589-38-8, 3-Hexanone 590-18-1, cis-2-Butene 590-21-6, 1-Chloropropylene 591-97-9, 1,4-Hexadiene 592-84-7, Butylformate 593-53-3, Methyl fluoride 593-60-2, Vinylbromide 624-64-6, trans-2-Butene 594-36-5, Tert Amyl chloride 624-64-6, Chlorofluoromethane 627-27-0, 3-Buten-1-ol 628-12-0, Ethylpropyl ether 628-63-7, Amyl acetate 821-55-6, Methylheptylketone 1067-20-5, 3,3-Diethylpentane 1321-74-0, Divinylbenzene, reactions 1331-43-7, Diethylcyclohexane 1640-89-7, Ethylcyclopentane 1653-19-6, 2,3-Dichlorobutadiene-1,3 1678-91-7, Ethylcyclohexane 1717-00-6, 1-Fluoro-1,1-dichloroethane 3266-23-7, 2,3-Butylene oxide 4170-30-3, Crotonaldehyde 4461-41-0, 2-Chloro-2-butene 4784-77-4, Crotyl bromide 4806-61-5, Ethylcyclobutane 6117-91-5, Crotonyl alcohol 7154-79-2, 2,2,3,3-Tetramethylpentane 12002-48-1, Trichlorobenzene 25013-15-4, Vinyltoluene 25167-70-8, 2,2,4-Trimethylpentane 25551-13-7, Trimethylbenzene 25561-67-3, Dinitrochlorobenzene 26519-91-5, Methylcyclopentadiene 26635-63-2, Sec Amyl alcohol 31394-54-4, Isobutane 62309-51-7, Propanol or reagent 80466-34-8, 2,4-Hexadienal R1: RCT (Reactant); RACT (Reactant or reagent)

REFERENCE COUNT: 7

(Prediction of flammability of gases by using F-number anal.)

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 32 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:13566 HCAPLUS Full-text
DOCUMENT NUMBER: 130:143189

TITLE: POCP for individual VOC under European conditions

AUTHOR(S): Alenstedt, Johannes; Plaijdel, Karin

CORPORATE SOURCE: Goteborg, Swed.

SOURCE: IVL Report (1998), B 1305, 1-47

CODEN: IVLBDO; ISSN: 0347-8696

DOCUMENT TYPE: Report

LANGUAGE: English

AB Entered STN: 11 Jan 1999

03 production from volatile organic compds. (VOC) in the atmospheric is discussed, focusing on a general way to present photochem. O3 creation potential (POCP) values for different VOC under European conditions and to calculate such values for a large number of VOC. Topics discussed include: environmental impact of VOC in atmospheric tropospheric O3; the photo-stationary state; NOx and VOC precursors of tropospheric O3; atmospheric chemical of VOC; ranking VOC according to their ability to produce O3; methods for critical anal. of POCP concept; results from critical anal. of the POCP concept; selecting model set-up to calculate POCP; POCP under European conditions; and conclusions.

IT 78-79-5, Isoprene, reactions 79-20-9, Methylacetate 123-86-4, n-Butylacetate 141-78-6, Ethylacetate, reactions R1: POL (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or reagent) (modelling photochem. ozone creation potentials and air pollution for individual volatile organic compds. in troposphere of Europe)

RN 78-79-5 HCAPLUS

CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)

RN 79-20-9 HCAPLUS

CN Acetic acid, methyl ester (CA INDEX NAME)

RN 123-86-4 HCAPLUS

CN Acetic acid, butyl ester (CA INDEX NAME)

n-Bu-O-Ac

RN 141-78-6 HCAPLUS

CN Acetic acid ethyl ester (CA INDEX NAME)

Et-O-Ac

CC 59-2 (Air Pollution and Industrial Hygiene)

Section cross-reference(s): 53

IT
Alcohols, reactions
Aldehydes, reactions
Alkenes, reactions
Alkynes
Aromatic compounds
Bases, reactions
Ketones, reactions
Rt: POL (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or reagent)
(modeling photochem. ozone creation potentials and air pollution for individual volatile organic compds. in troposphere of Europe)

50-00-0, Formaldehyde, reactions 60-29-7, Diethylether, reactions 64-17-5, Ethanol, reactions 64-19-7, Acetic acid, reactions 67-56-1, Methanol, reactions 71-36-3, Isopropanol, reactions 71-43-2, Benzene, reactions 71-55-6, 1,1,1-Trichloroethane 74-82-8, Methane, reactions 74-84-0, Acetylene, reactions 74-85-1, Ethene, reactions 74-86-2, 74-98-6, Propene, reactions 75-07-0, Acetaldehyde, reactions 75-18-3, Dimethyl sulfide 75-28-5, Isobutene, reactions 78-18-4, Isopentane 78-35-4, 1,1-Dichloroethene, reactions 78-84-2, Isobutylaldehyde 78-85-3, Methacrolein 78-93-3, Ethyl methyl ketone, reactions 78-98-8, Methylglyoxal 79-01-6, Trichloroethene, reactions 79-20-9, Methylacetate 95-47-6, 3-Methylpentane 98-82-8, Isopropylbenzene 100-41-4, Ethylbenzene, reactions 100-42-5, Styrene, reactions 100-52-7, Benzaldehyde, reactions 103-65-1, n-Propylbenzene 105-46-4, sec-Butylacetate 106-42-3, p-Xylene, reactions 106-97-8, Butane, reactions 106-98-9, 1-Butene, reactions 107-01-7, 2-Butene 107-02-8, Acrolein, reactions 107-06-2, 1,2-Dichloroethane, reactions 107-22-2, Glyoxal 107-83-5, m-Xylene, reactions 108-10-1, Methyl isobutyl ketone 108-38-3, 108-87-2, Methylcyclohexane 108-88-3, Toluene, reactions 109-66-0, Pentane, reactions 109-67-1, 1-Pentene 109-68-2, 2-Pentene 110-34-3, Hexane, reactions 110-62-3, Valeraldehyde 111-63-9, Octane, reactions 111-84-2, Nonane 112-40-3, Dodecane 113-07-1, Propene, reactions 115-10-6, Dimethylether 115-11-7, Iso-butene, reactions 123-38-6, Propionaldehyde, reactions 123-72-8, Butyraldehyde 123-86-4, n-Butylacetate 124-18-5, Decane 127-18-4, Tetrachloroethene, reactions 141-78-6, Ethylacetate, reactions 142-82-5, Heptane, reactions 513-35-9, 2-Methyl-2-butene 536-73-8, 1,2,3-Trimethylbenzene 563-46-2, 2-Methyl-1-butene 592-27-8, 2-Methylheptene 611-14-3, o-Ethyltoluene 620-14-4, m-Ethyltoluene 622-96-8, p-Ethyltoluene 624-92-0, Dimethyl disulfide 630-08-0, Carbon monoxide, reactions 871-83-0, 2-Methylnonane 1120-21-4, Undecane 1534-04-4, Methyl tertbutyl ether 3221-61-2, 2-Methyloctene 6975-98-0, 2-Methyldecane Rt: POL (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or reagent)
(modeling photochem. ozone creation potentials and air pollution for individual volatile organic compds. in troposphere of Europe)

REFERENCE COUNT: 42

THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 33 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:352465

DOCUMENT NUMBER: 127:17819

Study on CuCl₂ catalyzed hydrochlorination of myrcene. (III). Esterification of alkyl-type chlorides

AUTHOR(S): LI, Qianhe; Yin, Dulin
Institute Fine Catalysts Synthesis, Hunan Normal Univ., Changsha, 410081, Peop. Rep. China

SOURCE: Linchen Huaxue Yu Gongye (1997), 17(1), 16-20

PUBLISHER: CODEN: LHYGDT; ISSN: 0253-2417

LANGUAGE: Linchen Huaxue Yu Gongye Bianji Weiyuanhui Journal Chinese

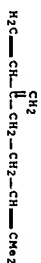
ED Entered STN: 05 Jun 1997

AB The esterification of linallyl, geranyl and neryl chlorides with NaOAc was studied. Effects of catalysts, reaction temperature and the compns. of hydrochlorides on the distribution of esters were investigated in detail. Results showed that all three allyl-type chlorides can be esterified with sodium acetate in acetic acid to yield linallyl acetate with 96% or more selectivity when catalyzed by CuCl₂. In the presence of Et₃N, the three allyl-type chlorides were converted to their acetates resp. linallyl acetate can be obtained with 96.5% selectivity under the optimum conditions.

IT 123-35-3, Myrcene 127-09-3, Sodium acetate Rt: RCT (Reactant); RACT (Reactant or reagent)

(specific chloride catalyzed hydrochlorination of myrcene and esterification of alkyl-type chlorides)

RN 123-35-3 HCAPLUS 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



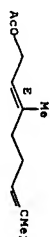
RN 127-09-3 HCAPLUS Acetic acid, sodium salt (1:1) (CA INDEX NAME)



Na

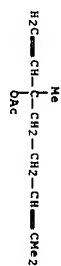
IT 105-87-3p, Geranyl acetate 115-95-7p, linallyl acetate 141-12-8p, Neryl acetate Rt: SPN (Synthetic preparation); PREP (Preparation) (specific chloride catalyzed hydrochlorination of myrcene and esterification of alkyl-type chlorides)

RN 105-87-3 HCAPLUS 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)



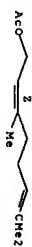
Double bond geometry as shown.

RN 115-95-7 HCAPLUS
CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)



RN 141-12-8 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z) - (CA INDEX NAME)

Double bond geometry as shown.



CC 30-10 (Terpenes and Terpenoids)
IT 123-35-3, Myrcene 127-09-3, Sodium acetate
471-10-3, Linalyl chloride 5389-87-7, Geranyl chloride
20536-36-1, Neryl chloride

RL: RCT (Reactant); RACT (Reactant or reagent)

(cupric chloride catalyzed hydrochlorination of myrcene and esterification of alkyl-type chlorides)
IT 105-87-3P, Geranyl acetate 115-95-7P, Linalyl acetate 141-12-8P, Neryl acetate

RL: SPN (Synthetic preparation); PREP (Preparation)
(cupric chloride catalyzed hydrochlorination of myrcene and esterification of alkyl-type chlorides)

L74 ANSWER 34 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:62046 HCAPLUS Full-text
DOCUMENT NUMBER: 126:157642
TITLE: Research and development in synthesis of series fine chemicals from rosin and turpentine. IV. Synthesis of neryl and geranyl acetates

AUTHOR(S): Li, Qianhe; Yin, Dulin; Li, Haotao; Lin, Liden; Ma, Runei

CORPORATE SOURCE: Institute of Fine Catalysts and Synthesis, Hunan Teacher's University, Changsha, 410081, Peop. Rep. China

SOURCE: Hunan Shifan Daxue Zixun Xuebao (1996), 19(3), 34-37

PUBLISHER: CODEN: HSDXEL; ISSN: 1000-2537

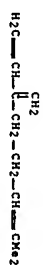
DOCUMENT TYPE: Journal

LANGUAGE: Chinese

ED Entered STN: 29 Jan 1997
AB Neryl and geranyl acetates were synthesized from β -pinene in turpentine oil by a 3-step process consisting of catalytic isomerization, hydrochlorination, and esterification. The effect of the esterification conditions on the yield of the title compds. was studied. In the presence of 28 EtSn (the catalyst) myrcene hydrochlorination crude products reacted with equimolar anhydrous NaOAc at 85-90° for 5 h, the total yield of the 2 title esters reached 66.6% based on β -pinene, in which ester products the selectivity of neryl acetate was 40-45% whereas that of geranyl acetate was 55-60%.

IT 123-35-3DP, Myrcene, hydrochlorination products
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)

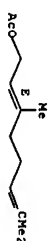


IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate

RL: SPN (Synthetic preparation); PREP (Preparation)

RN 105-87-3 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E) - (CA INDEX NAME)

Double bond geometry as shown.



RN 141-12-8 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z) - (CA INDEX NAME)

Double bond geometry as shown.



CC 30-10 (Terpenes and Terpenoids)
IT 123-35-3DP, Myrcene, hydrochlorination products

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

RN 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate

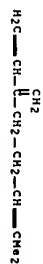
RL: SPN (Synthetic preparation); PREP (Preparation)
(β -pinene conversion to neryl acetate and geranyl acetate)

L74 ANSWER 35 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:74185 HCAPLUS Full-text
DOCUMENT NUMBER: 123:339558
TITLE: Tetracyanoethylene-hydrogen peroxide, a mild epoxidation system of olefins

AUTHOR(S): Masaki, Yukio; Miura, Tsuyoshi; Mukai, Isao; Iwata, Ichiro; Oda, Hirohisa; Itoh, Atsuhika
CORPORATE SOURCE: Gifu Pharmaceutical Univ., Gifu, 502, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1995), 43(4), 686-8

PUBLISHER: CODEN: CPBPAU; ISSN: 0009-2363
Pharmaceutical Society of Japan

RN	123-35-3	HCAPLUS
CN	1,6-Octadiene, 7-methyl-3-methylene-	(CA INDEX NAME



CC	30-1 (Terpenes and Terpenoids)	
	Section cross-reference(s): 5, 22	
IT	76-49-3, Bornyl acetate	79-92-5, Camphene
		80-56-8,

Myricene 127-91-3, β -pinene 138-66-3, limonene 44-48-2, (1S)-(-)-camphor 470-82-6, 1,8-Cineole 501-52-0, Hydrocarimide 2009-00-9, (+)-3-Terphenol 1135-27-6, Fenchic acid 1196-01-6, 2009-00-9, (+)-Sabinene 2244-14-8, (S)-(-)-Carvone 7764-50-1, 148486-69-6, (1R)-(-)-Myrtanol 19894-97-4, (1R)-(-)-Myrtanol 12267-22-1, 32719-61-2, Epiandroone 113412-11-6, Calamantrene 1135459-80-9, Desacetylcalamantrene 1135459-80-9, Reactant or reagents (water solubility of, determination of, via gas chromatog.).

L74 ANSWER 37 OF 67 HCAPLUS COPYRIGHT 2007 ACS on SNN
ACCESSION NUMBER: 1991:164539 HCAPLUS Full-text
DOCUMENT NUMBER: 114:164539
TITLE: Reductive radical cyclizations

AUTHOR(S) :

CORPORATE SOURCE:

SOURCE: Helvetica Chimica Acta (1991), 74, 1453.

74(1), 146-62
CONF. UCACTV. TCCU. 0018-018X

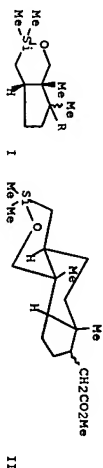
DOCUMENT TYPE.

DOCUMENT LIFE:

OTHER SOURCE(S):

ED Entered STN

19

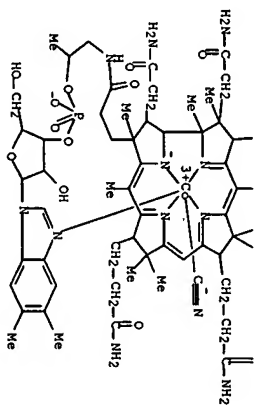
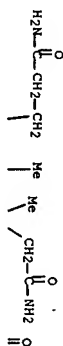


AB The tin hydride promoted and the reductive vitamin B12 catalyzed radical cyclization of mixed 2-bromoacetaldehyde acetals and of (2-bromomethyl)dimethylsilyl ethers of allylicisoterprenoid alcohols was investigated: 3-oxodeca-5,9-dien-1-yl radicals undergo 5-exo-cyclization to oxolanes, 3-oxa-2-siladeca-5,9-dien-1-yl radicals sequential 6-endo-5-

IT 68-19-9, Vitamin B12

IT	68-19-9, Vitamin B12
	RI: RCF (Reactant); RACT (Reactant or reagent) (catalyst for reductive radical cyclization of terpenoids; bromoacetal or bromomethylsilyl ether)
RN	68-19-9 HCAPUS
CN	Vitamin B12 (CA INDEX NAME)

PAGE 1-A



PAGE 2-4

IT 105-45-3, Methyl acetoacetate

RL: RCT (Reactant); RACT (Reactant or reagent)
(dianion alkylation of, with siloxygeranyl bromide)

RN	105-45-3	HCAPLUS
CN	Butanoic acid, 3-oxo-, methyl ester	(CA INDEX NAME)

CN Butanoic acid, 3-oxo-, methyl ester (CA INDEX NAME

DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 123-339558
 ED Entered STN: 17 Aug 1995
 GI



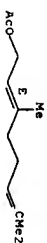
AB A reagent combination system, tetraacetoethylene (1)-10% H2O2, epoxidized olefins efficiently in MeCN at room temperature in a stereospecific manner with retention of the configuration of the double bond. H2O2 30% was added to I and cis-3-hexen-1-ol in MeCN at room temperature for 12 h to give cis-II.

IT 105-87-3 123-35-3 540-88-5, tert-Butyl acetate
 RL: RCT (Reactant); RACT (Reactant or reagent)

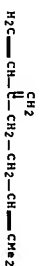
(tetraacetoethylene-hydrogen peroxide, a mild epoxidn. system of olefins)

RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 123-35-3 HCAPLUS
 CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



RN 540-88-5 HCAPLUS
 CN Acetic acid, 1,1-dimethylethyl ester (CA INDEX NAME)



CC 27-2 (Heterocyclic Compounds (One Hetero Atom))
 IT 105-87-3 106-23-0 106-24-1 108-98-5, Benzenethiol, reactions 110-93-0 123-35-3 540-88-5, tert-Butyl acetate 870-63-3, 1-bromo-3-methyl-2-butene 928-96-1, cis-3-hexen-1-ol 3695-38-3 42272-94-6 42602-37-9 51113-72-5 52188-73-5 76871-78-8 88191-39-3
 RL: RCT (Reactant); RACT (Reactant or reagent) (tetraacetoethylene-hydrogen peroxide, a mild epoxidn. system of olefins)

174 ANSWER 36 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1994-8750 HCAPLUS Full-text
 DOCUMENT NUMBER: 120-8750
 TITLE:
 AUTHOR(S):
 CORPORATE SOURCE:
 SOURCE:
 CODEN: JCECD8; ISSN: 0098-0331
 19(8), 1799-807
 Journal of Chemical Ecology (1993),
 19(8), 1799-807

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 08 Jan 1994

AB Prior generalizations about the ecol. roles of monoterpenes may be misleading if based on the presumed insol. of monoterpenes in water. The authors determined the aqueous solubility of 31 biol. active monoterpenes by gas chromatog. While hydrocarbons were of low solubility (<35 ppm), oxygenated monoterpenes exhibited solubilities one or two orders of magnitude higher, with ranges of 155-6990 ppm for ketones and of 183-1560 ppm for alcs. Many monoterpenes are phytotoxic in concns. under 100 ppm, well below the saturated aqueous concns. of oxygenated monoterpenes. Therefore, even dilute, unsatd. solns. of monoterpenes, occurring naturally in plant tissues and soil solns., may act as potent biol. inhibitors.

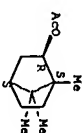
IT 76-49-3, Bornyl acetate 105-87-3, Geranyl acetate 115-95-7, Linalyl acetate 123-35-3, Myrcene

RL: RCT (Reactant); RACT (Reactant or reagent)

(water solubility of, determination of, via gas chromatog.)

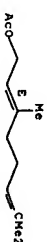
RN 76-49-3 HCAPLUS
 CN Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, 2-acetate, (1R,2S,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.

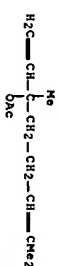


RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

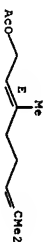


RN 115-95-7 HCAPLUS
 CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)



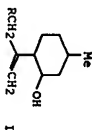
$$\text{H}_3\text{C}-\overset{\text{CH}_2}{\underset{\text{CH}_2}{\text{C}}}=\text{CH}_2$$

Double bond geometry as shown.

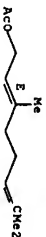


L74 ANSWER 38 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:459553 HCAPLUS Full-text

Page 93



Double bond geometry as shown.


$$\text{H}_2\text{C}=\text{CH}-\overset{\text{CH}_2}{\underset{|}{\text{C}}}-\text{CH}_2-\text{CH}=\text{CH}_2$$

Page 94

LANGUAGE: Chinese

ED Entered STN: 12 Jan 1991

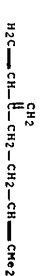
AB The synthetic route of geraniol and nerol was studied. Myrcene which was obtained from p-phenylene in gum turpentine by heat isomerization was used as raw material. In the presence of catalyst, myrcene was treated by addition of HCl to form an adduct mixture consisting mainly of geranyl chloride and neryl chloride with small amounts of other chlorides such as linalyl chloride and turpene chloride present. These then converted sep. to their resp. acetate esters by treatment with sodium acetate in the presence of a catalyst. The major products are geranyl acetate and neryl acetate. The yield of the acetates was 50-60%, and the ratio of geranyl acetate to neryl acetate in the mixed reaction time were investigated. Saponification of the acetates produced the resp. alcs. Pure geraniol and nerol were separated by rectification on a highly efficient packed column.

IT 123-35-3, Myrcene

RL: RCT (Reactant); RACT (Reactant or reagent)

CN 123-35-3, Myrcene

CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



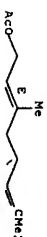
IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

IT 105-87-3, Geranyl acetate 141-12-8P, Neryl acetate

Double bond geometry as shown.



RN 141-12-8, HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.



CC 30-10 (Terpenes and Terpenoids)

IT 123-35-3, Myrcene

RL: RCT (Reactant); RACT (Reactant or reagent)

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate

(Preparation and saponification of)

L74 ANSWER 40 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1989:439594 HCAPLUS Full-text
DOCUMENT NUMBER: 111:39594

TITLE: The regioselectivity of elimination reactions in terpene derivatives

AUTHOR(S): Badet, B.; Julia, M.; Mallet, J. M.; Schmitz, C.

CORPORATE SOURCE: Lab. Chim., Ec. Norm. Supér., Paris, 75231, Fr.

SOURCE: Tetrahedron (1988), 44(10), 2913-24

CODEN: TETRA; ISSN: 0040-4020

DOCUMENT TYPE: Journal

OTHER SOURCE(S): CASREACT 111:39594

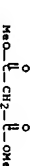
AB Tertiary alcs. with prenyl or geranyl moieties, bearing a second oxygen function in the 3, 4 or 5 position were dehydrated under various conditions: the composition of the olefinic mixture obtained was accounted for, by an intramol. base relay effect. Basic elimination of analogous dimethylsulfonium salts gave results that could be related to the inductive effect: a correlation between regioselectivity and the Taft constant of the second oxygen function was found, except for the very basic alkoxide groups where an alternative regioselective elimination took place.

IT 108-59-8, Dimethyl malonate

RL: RCT (Reactant); RACT (Reactant or reagent)

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

IT 108-59-8, Dimethyl malonate

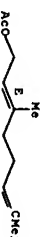


IT 105-87-3P 141-12-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

RN 105-87-3, HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.



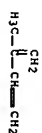
RN 141-12-8, HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.



$$\text{AcO}-\text{CH}_2-\text{CH}=\text{CH}_2$$

IT	78-79-5, Isoprene, reactions
	RL: RCT (reactant); PACT (reactant or reagent)
	(reaction of, dimethylsulfide, sulfonium salt from)
RN	78-79-5 HCAPUS
CN	1,3-Butadiene, 2-methyl- (CA INDEX NAME)



CC	30-10 (Terpenes and Terpenoids)
IT	Section cross-reference(s): 22
	108-59-8, Dimethyl malonate

RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation of, by prenyl bromide or tosylate)

455-58-1P	3233-35-8P	3229-37-0P	5944-20-7P	6819-38-1P
7733-91-7P	13066-51-8P	20776-25-1P	27557-00-4P	40121-12-8P
53840-11-2P	55029-75-3P	65947-42-6P	65343-20-4P	
69301-53-7P	65301-54-8P	71724-57-7P	72858-60-7P	
74780-61-3P	77958-38-4P	100659-16-7P	100659-17-8P	
107657-13-2P	107657-15-7P	107657-32-1P	107657-29-0P	
121402-99-1P	121403-00-7P	121403-01-8P	121403-02-9P	
121403-03-0P	121403-17-6P	121403-15-9P	121403-21-2P	
121403-22-3P	121403-43-4P	121403-28-1P	121403-27-8P	
121403-28-9P	121403-29-0P	121403-30-2P	121403-31-4P	
121403-32-5P	121403-33-6P	121403-34-7P	121403-35-8P	
121403-36-9P	121403-37-0P			

RI: SPN (Synthetic Preparation), PREP (Preparation)

IT	556-82-1P	753-89-3P	929-12-9P	1191-18-6P	
	1589-86-4P	14309-13-0P	1699-86-5P	15162-00-6P	22094-02-6P
	15901-76-9P	88632-02-4P	88632-76-0P	88656-78-7P	
RI: SPN	(Synthetic preparation);	PREP	(Preparation of, via dehydration of tertiary terpene alcs.)		
IT	78-79-5				
	Isoprene, reactions				
RI: RCT	(Reactant);	RACT	(Reactant or reagent)		
	(reaction of, dimethylsulfide, sulfonium salt from)				

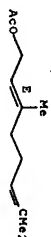
L74 ANSWER 41 OF 67 HCAPUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1999-633218 HCAPUS Full-text
 DOCUMENT NUMBER: 111-233218
 TITLE: Allylic chlorination of isoprenoid
 oligoolefins with sulfuryl chloride
 Veselovski, V. V.; Dragan, V. A.; Gelfirov, N.
 AUTHOR(S):

CORPORATE SOURCE: Inst. Org. Khim. im. Zelinskogo, Moscow, USSR
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya khim. nauk, 1980, No. 1, p. 100.

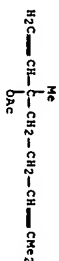
[illegible]

NAME	CA INDEX	REAGENT OR REAGENT	REAGENT OR REAGENT
105-87-3	HCAPLUS	allicyl chlorination of,	by sulfonyl chloride)
2,6-Octadecen-1-ol,	3,7-dimethyl-,	1-acetate,	(2E)-

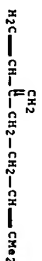
Double bond geometry as shown.



RN	115-95-7	HCAPLUS
CN	1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate	(CA INDEX NAME)



RN	123-35-3	HCAPLUS
CN	1,6-Octadiene, 7-methyl-3-methylene-	(CA INDEX NAME)



RN	HCAPLUS	CA INDEX
CN	141-12-8	2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)-
	(NAME)	

Double bond geometry as shown.



RN	150-84-5	HCAPLUS
CN	6-Octen-1-ol, 3,7-dimethyl-, 1-acetate	(CA INDEX NAME)



CC 30-10 (Terpenes and Terpenoids)
IT 105-87-3 115-95-7 123-35-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(allylic chlorination of, by sulfoxyl chloride)

174 ANSWER 42 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1989-534484 HCAPLUS Full-text
DOCUMENT NUMBER: 111:134484

TITLE: Reaction of sulfoxide hydrochlorides and hydrobromides with trisubstituted olefins
Moiseenkov, A. M.; Dragan, V. A.; Lozova, A. V.; Veselovskii, V. V.

CORPORATE SOURCE: Inst. Org. Khim. Im. Zelinskogo, Moscow, USSR
Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1988), (8), 1797-803

CODEN: IASRA6; ISSN: 0002-3353

LANGUAGE: Russian
JOURNAL

OTHER SOURCE(S): CASREACT 111:134484

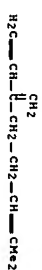
ED Entered STN: 14 Oct 1989

AB Chlorination of Me₂C(CH₂CH₂CH₂C(X)Me (X = H, OMe, H, CH₂CH₂OMe; CHCH₂OMe) by RI₂SO₂ HCl (R = Me, Ph, R₁₂ = (CH₂)₄) in MeNO₂ or CH₂Cl₂ containing CH₂OMeCH₂CH₂CH₂CH₂C(X)Me, CCl₄ at -50° or by HCl-AcOH at 0° gave mixts. containing CH₂OMeCH₂CH₂CH₂CH₂C(X)Me, Me₂CCl(CH₂)₃C(X)Me, and Me₂CClCH₂CH₂CH₂C(X)Me whose yields and ratios depended on the process. Addnl. obtained were some bromo derivs.

IT 123-35-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination of)

RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)

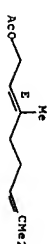


IT 105-87-3 150-84-5

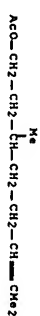
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination and bromination of, by sulfoxide hydrochlorides and hydrobromides)

RN 105-87-3 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 150-84-5 HCAPLUS
CN 6-Octen-1-ol, 3,7-dimethyl-, 1-acetate (CA INDEX NAME)



CC 30-10 (Terpenes and Terpenoids)
IT 123-35-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination of)

IT 105-87-3 150-84-5 19162-00-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination and bromination of, by sulfoxide hydrochlorides and hydrobromides)

174 ANSWER 43 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988-493347 HCAPLUS Full-text
DOCUMENT NUMBER: 109:93347

TITLE: Regiospecific ene-type reaction of benzenesulfinyl chloride with linear isoprenoids
Veselovskii, V. V.; Dragan, V. A.; Moiseenkov, A. M.

CORPORATE SOURCE: Inst. Org. Khim. Im. Zelinskogo, Moscow, USSR
Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1987), (12), 2787-90

CODEN: IASRA6; ISSN: 0002-3353

LANGUAGE: Russian
JOURNAL

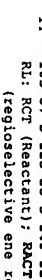
OTHER SOURCE(S): CASREACT 109:93347

ED Entered STN: 17 Sep 1988
AB Treating RCH=CMe₂ (R = CH₂CH₂C(CH₂)CH₂CH₂OMe; trans- and cis-CH₂CH₂OMe; CHCH₂OMe; CHCH₂OMe; CHCH₂OMe; CHCH₂OMe) with PhSOCl in Me₂CHNO₂ containing ZnCl₂ gave 50-65% PhSOCH₂CH₂OMe:CH₂ (I) which underwent a sulfoxide-sulfonate rearrangement in the presence of P(OMe)₃-MeOH to give 85-90% E-RCH=CMeCH₂OMe. Grignard reaction of I (R = CH₂CH₂C(CH₂)CH₂CH₂OMe) with Me₂C=CHCH₂CH₂OMe in the presence of CuI-TfH gave 34% of a 4:1 E/Z mixture of Me₂C=CHCH₂CH₂OMe:CHCH₂CH₂OMe:CHCH₂CH₂OMe.

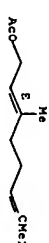
IT 105-87-3 123-35-3 141-12-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(regioselective ene reaction of, with benzenesulfinyl chloride)

RN 105-87-3 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)



Double bond geometry as shown.



RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



RN 141-12-8 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z) - (CA INDEX NAME)

Double bond geometry as shown.



CC 30-15 (Terpenes and Terpenoids)
IT 105-87-3 123-35-3 141-12-8
19954-66-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(regioselective ene reaction of, with benzenesulfinyl chloride)

L74 ANSWER 44 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:510661 HCAPLUS Full-text
DOCUMENT NUMBER: 109:110661
TITLE: Regioselective ene reaction of benzenesulfinyl chloride with linear isoprenoids

AUTHOR(S):

Moiseenko, A. M.; Dragan, V. A.; Koptenkova, V. A.; Veselovskii, V. V.

CORPORATE SOURCE: N. D. Zelinskii Inst. Org. Chem., Moscow, USSR

SOURCE: Synthesis (1987), (9), 814-15
CODEN: SYNTHF; ISSN: 0039-7881

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:110661

ED Entered STN: 01 Oct 1988

AB The Lewis acid (e.g., ZnCl₂) catalyzed ene reaction of PhSOCl with myrcene, geranyl and neryl acetates, as well as Et (E)-farnesate proceeds smoothly and chemoselectively by exclusive attack at the terminal trisubstituted C:C bond to give allylic sulfonates.

IT 105-87-3, Geranyl acetate 123-35-3, Myrcene

141-12-8, Neryl acetate

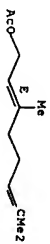
RL: RCT (Reactant); RACT (Reactant or reagent)

(ene reaction of, with benzenesulfinyl chloride)

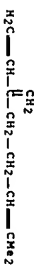
RN 105-87-3 HCAPLUS

CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E) - (CA INDEX NAME)

Double bond geometry as shown.



RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



RN 141-12-8 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z) - (CA INDEX NAME)

Double bond geometry as shown.



CC 30-10 (Terpenes and Terpenoids)
IT 105-87-3, Geranyl acetate 123-35-3, Myrcene
141-12-8, Neryl acetate 19954-66-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(ene reaction of, with benzenesulfinyl chloride)

L74 ANSWER 45 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:481183 HCAPLUS Full-text
DOCUMENT NUMBER: 105:81183
TITLE: Tertiary, optionally halogenated allylic esters

INVENTOR(S):

Mulhauser, Michel

PATENT ASSIGNEE(S):

Rhone-Poulenc Sante, Ft.

SOURCE: Eur. Pat. Appl., 16 pp.

DOCUMENT TYPE: Patent

FAMILY ACC. NUM. COUNT: 2

LANGUAGE: French

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 179685	A1	19860430	EP 1985-401819	1985 0919

EP 179685	B1	19880928		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
FR 2570374	A1	19860321	FR 1984-14427	1984 0920

FR 2570374	B1	19871224	FR 1985-3841	1985 0315
FR 2578840	A2	19860919		

FR 2578840	B2	19881007	AT 1985-401819	1985 0919
AT 37532	T	19881015		

PRIORITY APPL. INFO.:
FR 1984-14427 A 1984 0920
FR 1985-3841 A 1985 0315
EP 1985-401819 A 1985 0919

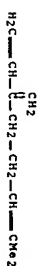
ED Entered STN: 06 Sep 1986

AB A method is described of manufacturing a tertiary, optionally halogenated allylic ester by the reaction of an alkali metal salt of a carboxylic acid with a primary and/or tertiary allylic halide (prepared by hydrohalogenation of an optionally halogenated polyene containing 2 conjugated double bonds and, optionally, 21 more double bond). The hydrohalogenation catalyst is composed of a Cu(I) salt (e.g., CuI or CuCl), an ammonium salt (e.g., tetraalkylammonium halide or trialkylamine hydrohalide) or a phosphonium salt (e.g., tetraalkyl phosphonium halide). The starting polyene is chosen from myrcene, β -farnesene, β -spergine, phytatriene and phytatetraene. Thus, in a reactor under Ar were combined 330 mL CH₂Cl₂, Et₃N-HCl 3.33, CuCl 2.4, and myrcene 164.4 g. The reaction mixture was cooled to -5° and 43 g HCl was added. After the hydrochlorination step, the solution was added to another reactor, under Ar, containing anhydrous NaOAc 145, CuCl 2.4, and Et₃N-HCl 3.3 g. CuCl 2.4 g was added and the solution was mixed 18 h at 20°. The reaction mixture was cooled and an intensely blue aqueous phase and a clear brown organic phase were obtained. After decanting, the 200 mL H₂O and dried with K₂CO₃. After filtration and solvent evaporation, an oil 237.1 g was obtained, containing 59% linallyl acetate. The yield from myrcene was 84.5%. The selectivity for linallyl acetate, expressed as the ratio of linallyl acetate to the sum of linallyl acetate, geranyl acetate, and neryl acetate, was 97%.

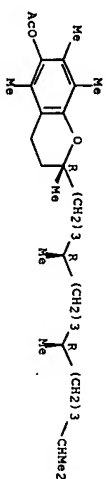
IT 127-09-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(acetoxylation by, of hydrohalogenated polyenes)
RN 127-09-3 HCAPLUS
CN Acetic acid, sodium salt (1:1) (CA INDEX NAME)



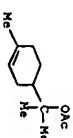
IT 123-35-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrohalogenation of, copper halide-quaternary ammonium salt
or phosphonium salt-catalyzed)
RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



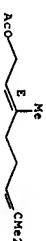
IT 58-95-7P
RL: PREP (Preparation)
(manufacture of, by hydrogenation)
RN 58-95-7 HCAPLUS
CN 2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-[(4R,8R)-4,8,12-trimethyltridecyl]-, 6-acetate, (2R)- (CA INDEX NAME)
Absolute stereochemistry.



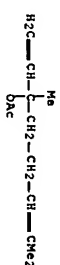
IT 80-26-2P 105-87-3P 115-95-7P
141-12-8P
RL: PREP (Preparation)
(manufacture of, copper chloride-triethylamine hydrochloride-
catalyzed)
RN 80-26-2 HCAPLUS
CN 3-Cyclohexene-1-methanol, α,α,δ -trimethyl-, 1-acetate
(CA INDEX NAME)



RN 105-87-3 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)
Double bond geometry as shown.



RN 115-95-7 HCAPLUS
CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)



RN 141-12-8 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)
Double bond geometry as shown.



IC ICM C07C067-11
ICS C07C068-145; C07C069-63
ICA C07C017-02; C07C021-04
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 67
Esters, preparation
IT

(branched, β - γ -unsatd., manufacture of, from
hydrohalogenated polyenes, copper halide- and quaternary
ammonium or phosphonium salt-catalyzed)

IT	123-35-3	18794-84-8	70901-63-2	71138-26-6
RL:	RCT (Reactant); RACT (Reactant or reagent)			
	(acetoxylation by, of hydrohalogenated polyenes)			

RL: RCT (Reactant); RACT (Reactant or Reagent)
(hydrohalogenation of, copper halide-quaternary ammonium salt)
or phosphonium salt-catalyzed)

RL: PREP (Preparation)
 (manufacture of, by hydrogenation)
 IT 80-26-22 105-87-3P 115-95-7P
 141-12-8P 1118-39-4P
 RL: PREP (Preparation)
 (manufacture of, copper chloride-triethylamine hydrochloride-catalyzed)

L74 ANSWER 46 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STT
ACCESSION NUMBER: 1986:6049 HCAPLUS Full-text
DOCUMENT NUMBER: 104:6049
TITLE: Regio- and stereoselective term

AUTHOR(S): Synthesis of biologically important linear degraded terpenoids
Matsuda, Yukio, Sakuma, Kazuhiko, Kaji, Kenji
CORPORATE SOURCE: Gifu Coll. Pharm., Gifu, 502, Japan
CONTRACT NUMBER: Chemical & Pharmaceutical Bulletin (

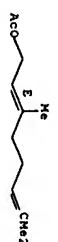
DOCUMENT TYPE: CODEN: CPBIAL; IS
LANGUAGE: Journal
OTHER SOURCE(S): English
ED Entered STN: CASREACT 104:6049
G1 11 Jan 1986

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT

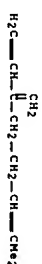
gem-Di-Meoxalifins, e.g., I (R = O (R1 = PhCH₂, AcO, MeOCH₂), O1 (R2 = MeO, R3 = PhCH₂, Me, n = 0,1) were regioselectively converted to the sulfides II via addition of MeOCH₂CHSCl followed by dehydrochlorination, or chlorination with SOCl₂ followed by sulfenylation with MeOCH₂CH₂SH. Treatment of II with MeOK or NaH in DMF and DMSO gave esters III by stereoselective desulfurative [2,3]-sigmatropic rearrangement. Ester IV, a component of the pheromonal secretion of the queen butterfly, and quinoxid acids V (R2, as above, m = 1,2), metabolites of polycycloprenoid quinones, were prepared by this method.

IT	105-87-3	123-35-3	
	RL: RCT (Reagent); RACT (Reactant or reagent)		
	(chlorination and chlorosulfonylation of)		
RN	105-87-3	HCAPIUS	
CA	2,6-octadecan-1-ol, 3,7-dimethyl-, 1-acetate, (2E)-		(CA INDEX NAME)

Double bond geometry as shown.



RN	HCAPLUS
CN	1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



IT	2365-48-2	RL: RCP (Reactant); RACT (Reactant or reagent) (chlorination and reaction of, with methyl) chlorides
RN	2365-48-2	HCAPUS.
CN	Acetic acid, 2-mercapto-, methyl ester (CA INDEX NAME)	



CC	30-40	(Terpenes and Terpenoids)	
IT	105-87-3	123-35-3	4957-17-9 32347-33-9
	52288-77-5	53772-25-1	65586-67-6 70473-30-2
	83036-57-1	99347-48-5	
	RL: RCT (Reactant); PACT (Reactant or reagent)		
	(chlorination and chlorosulfenylation of)		
IT	2365-48-2		83036-56-0

L74 ANSWER 47 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1986:6027 HCAPLUS Full-text
 DOCUMENT NUMBER: 104:6027
 TITLE: Study on the regioselectivity of subst
 N,N'-KCl (reagent); NAl (reagent or reagent)
 (chlorination and reaction of, with methylal chlorides

TITLE: Study on the regioselectivity of substitution of carbonbons by allylic derivatives catalyzed by palladium. Selective preparation of compounds with quaternary carbon

AUTHOR(S): Cuvigny, Therese; Julia, Marc; Rolando, C.

CORPORATE SOURCE: Lab. Chim., Ec. Norm. Supér., Paris, 75231/05.

SOURCE: Journal of Organometallic Chemistry
DOCUMENT TYPE: 1885, 285(1-3), 395-413
CODEN: JORCAI; ISSN: 0022-328X
LANGUAGE: French
OTHER SOURCE(S): CASREACT 104:6027

AB The influence of the leaving groups, carbonions and ligands on π -allylpalladium has been investigated in the substitution of primary or tertiary (eicene derivs., β -9'-germyl acetate, neryl acetate. Conditions have been found under which the substitution takes place essentially at one or the other end of the allylic system. This provides a new and convenient way to obtain compds. with quaternary C's, which have been exemplified by the synthesis of $\text{CH}_2\text{:CHCH}_2\text{C(CH}_3)_2\text{CH}_2\text{CN}$.

(catalysts, containing palladium, for substitution of carbanions by allylic derivatives)

IT 105-87-3 115-95-7 141-12-8

72863-21-9 72863-23-1 99372-00-6

RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution by, of carbanions in presence of palladium)

L74 ANSWER 48 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985-95834 HCAPLUS Full-text

DOCUMENT NUMBER: 102:95834

benzenesulfonyl chloride addition

CORPORATE SOURCE:
Gifu Coll. Pharm., Gifu, 502, Japan

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal
LANGUAGE: English

ED	Entered SYN: 22 Mar 1985
AB	Addition reaction of RCH

(methylenedioxy)propyl, etc.] with PhSeCl gave the corresponding isomeric $\text{RCH}_2\text{CH}(\text{SPh})\text{CMe}_2\text{Cl}$ and $\text{RCH}_2\text{CHClCMe}_2\text{SPh}$. Hydrolysis in the presence of sil-

dehydrochlorination under neutral or weakly basic conditions, or dehydrochlorination under strongly basic conditions gave the hydroxy sulfides BCH2CH(SPh)CMe2OH.

methyllyc sulfides RCH₂CH(SPh)CMe:CH₂ (I), or vinyl sulfides RCH₂C(SPh):CMe₂, resp. I were converted to terminal trans-allyl sulfides RCH=CH-CMeCH₂SPh.

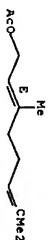
IT 105-87-3 115-95-7 123-35-3

RL: RCT (Reactant); RACT (Reactant or reagent

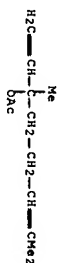
RN 105-87-3 HCAPLUS

LN	2, 6-OCLODIOLEIN-1-OL, 3, 7-DIMETHYL-, 1-ACETATE, (Z)-	100 INDEX
(NAME)		

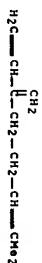
Double bond geometry as shown.



RN	115-95-7	HCAPLUS
CN	1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate	(CA INDEX NAME)



RN	123-35-3	HCAPLUS
CN	1,6-Octadiene, 7-methyl-3-methylene-	(CA INDEX NAME)

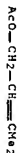


CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z) - (CA INDEX)

Double bond geometry as shown



RN	1191-16-8	HCAPLUS
CN	2-Buten-1-ol, 3-methyl-, 1-acetate	(CA INDEX NAME



CC	30-10 (Terpenes and Terpenoids)
IT	105-87-3 115-95-7 123-35-3

3695-38-3 22089-60-7 52188-73-5 5322

35032-55-4 88030-44-8 10413-30-2 10413-31-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(addition reaction of, with benzenesulfonyl chloride,

1985:62471 HCAPLUS Full-text
L74 ANSWER 49 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:

DOCUMENT NUMBER:
TITLE:

terpenoid allomones and pheromone components:

β -sprüngene

Renzo

CORPORATE SOURCE:
FAC, SCI. MFN, UNIV. PISA, PISA, I-56100/
Italy

SOURCE: Gazzetta Chimica Italiana (1964) 114(9-10), 443-9

DOCUMENT TYPE: Journal
CODEN: GCITA9; ISSN: 0016-5603

LANGUAGE: English
ED Entered STN. 24 Feb 1985



AB
Chemical and stereoisomerically pure dendroisoashin [I; R = (E)-O⁻ (R = MeC(CH₂CH₂CH₂CHMe)CH=CH₂) was prepared by Grignard reaction of I (R = Bz) with (E)-O-OOH in the presence of LiEtOCH₂F, whereas similar reaction of neryl acetate gave 9% stereoisomerically pure I (R = neryl). Moreover, β-farnesene [(E)-CH=CH₂(CH₂CH=CH₂) and β-sitosterol [(E,E)-CH₂=CH(CH₂CH=CH₂CH=CH₂CH=CH₂CH=CH₂CH=CH₂CH=CH₂)] were

IT	105-87-3	141-12-8	RL: RCT (Reactant); RACT (Reactant or reagent)
			(Originated reaction of, with (bromomethyl)furan)
	105-87-3	HOAPLUS	
CN	2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (ZE)-		(CA INDEX NAME)

CC(C)C/C=C/COC(=O)C

RN	HCAPLUS	CA INDEX
CN	141-12-8 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (NAME)	

CC=CC(C)C(=C)COCC

IT	123-35-3	
	RL: RCT (Reactant); RACT (Reactant or reagent)	
	(oxidation of)	
RN	123-35-3 HCAPIUS	
CN	1,6-Octadiene, 7-methyl-3-methylene-	(CA INDEX NAME)

$$\text{H}_2\text{C}=\text{CH}-\underset{\text{CH}_2}{\overset{\text{CH}_2}{\text{C}}}-\text{CH}_2-\text{CH}=\text{CH}_2$$

CC	30-20 (Terpenes and Terpenoids)
IT	105-87-9 141-12-8
	RL: RCT (Reactant); RACT (Reactant or reagent)
	(S ₂)-E ₂ reaction of, with (bromomethyl)luran
	123-35-3
IT	RL: RCT (Reactant); RACT (Reactant or reagent)
	RL: (oxidation of)

L74 ANSWER 50 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1993/454028 HCAPLUS Full-text
 DOCUMENT NUMBER: 99-54028
 TITLE: Allyl chlorides
 PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan
 SOURCE: Upr. Kodai Tokyo Kono, 3 pp.
 CODEN: JKOKXAF
 PATENT
 DOCUMENT TYPE: Japanese
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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Page 111

PRIORITY APPLN. INFO.: JP 1981-149226

AD Entered STN: 12 May 1984
 ED RCH2CH:CH:CH2 (R = terphenyl group) (I) were prepared by reaction of RCH2CH:CH:CH2CH2R1 and R2CH:CH:CH2 with trichloroisocyanuric acid. Thus, 15.0 g (R1 = H, Cl, OH, O2SC6H4-4-ep, O2SCH3) with trichloroisocyanuric acid was added to 39.20 g geranyl acetate in hexane over 30 min, the resulting mixture kept at -5 to 0° for 1 h, and more trichloroisocyanuric acid added at the same temperature until no more unreacted geranyl acetate was detected by gas chromatog. to give 43.53 g I (R = AcOCH2CH:CH:CH2).

RM	(chlorination of, by trichloroisocyanuric acid)
CN	105-87-3 HCAPLUS
NAME	2,6-Octadecen-1-ol, 3,7-dimethyl-, 1-acetate, (ZE)- [CA INDEX]

• Double bond geometry as shown.

CC(C)C/C=C/C(=C)COCC

RN	HCAPLUS	(CA INDEX NAME)
CN	1,6-Octadiene, 7-methyl-3-methylene-	

$$\text{H}_2\text{C}=\text{CH}-\overset{\text{CH}_2}{\underset{|}{\text{C}}}-\text{CH}_2-\text{CH}_2-\text{CH}=\text{CH}_2$$

RN	141-12-8	HCAPLUS
CN	2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)-	(CA INDEX NAME)

Double bond geometry as shown.

CCOC(=O)C/C=C/C(C)CC/C=C/C

L74 ANSWER 51 OF 67 HCAPLUS COPYRIGHT 2007 ACS ON STM
ACCESSION NUMBER: 1993:513189 HCAPLUS Full-text
(chlorination of, by trichloroacetic acid)

Page 112

PRIORITY APPLN. INFO.: JP 1981-149226

AD Entered STN: 12 May 1984
 ED RCH2CH:CH:CH2 (R = terphenyl group) (I) were prepared by reaction of RCH2CH:CH:CH2CH2R1 and R2CH:CH:CH2 with trichloroisocyanuric acid. Thus, 15.0 g (R1 = H, Cl, OH, O2SC6H4-4-ep, O2SCH3) with trichloroisocyanuric acid was added to 39.20 g geranyl acetate in hexane over 30 min, the resulting mixture kept at -5 to 0° for 1 h, and more trichloroisocyanuric acid added at the same temperature until no more unreacted geranyl acetate was detected by gas chromatog. to give 43.53 g I (R = AcOCH2CH:CH:CH2).

RM	(chlorination of, by trichloroisocyanuric acid)
CN	105-87-3 HCAPLUS
NAME	2,6-Octadecen-1-ol, 3,7-dimethyl-, 1-acetate, (ZE)- [CA INDEX]

• Double bond geometry as shown.

CC(C)C/C=C/C(=C)COCC

RN	HCAPLUS	(CA INDEX NAME)
CN	1,6-Octadiene, 7-methyl-3-methylene-	

$$\text{H}_2\text{C}=\text{CH}-\overset{\text{CH}_2}{\underset{|}{\text{C}}}-\text{CH}_2-\text{CH}_2-\text{CH}=\text{CH}_2$$

RN	141-12-8	HCAPLUS
CN	2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)-	(CA INDEX NAME)

Double bond geometry as shown.

CCOC(=O)C/C=C/C(C)CC/C=C/C

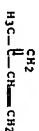
L74 ANSWER 51 OF 67 HCAPLUS COPYRIGHT 2007 ACS ON STM
ACCESSION NUMBER: 1993:513189 HCAPLUS Full-text
(chlorination of, by trichloroacetic acid)

Page 112

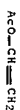
DOCUMENT NUMBER: 98:53189
 TITLE: Carboxylic acid esters
 INVENTOR(S): Schieppinoff, Bernhard; Leblanc, Hans;
 PATENT ASSIGNEE(S): Mallmann, Karl Heinz
 EC Erdelchemie G.m.b.H., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 38 pp.
 CODEN: GMMXBX
 PATENT: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3105399	A1	19821021	DE 1981-3105399	1981 0214
PRIORITY APPLN. INFO.: DE 1981-3105399				
Entered STN: 12 May 1984				

AB Acid ion exchangers, partially neutralized with cations (e.g., K, NH₄) were used as catalysts for addition of carboxylic acids to alkenes. Thus, 100 g Lewatit SPC 118 was treated with 13.7 g KCl in 200 mL H₂O to give a catalyst 45% neutralized. Data for runs with e.g., H₂OAc with EtOAc:CH₂: isoprene (to give prenyl acetate), or cyclopentadiene and EtOAc with styrene were given.
 IT 78-79-5, reactions 108-05-4, reactions
 R.I. RCT (Reactant); RACT (Reactant or reagent)
 RN 78-79-5 HCAPLUS (addition reaction of, with acetic acid, catalysts for)
 CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)

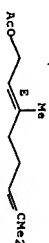


RN 108-05-4 HCAPLUS
 CN Acetic acid ethenyl ester (CA INDEX NAME)



IT 105-87-3P 141-12-8P 1191-16-8P
 R.I. SPN (Synthetic Preparation); PREP (Preparation)
 (Preparation of)
 RN 108-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.



RN 141-12-8 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)
 Double bond geometry as shown.



RN 1191-16-8 HCAPLUS
 CN 2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)



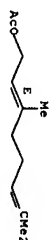
IC C07C067-04
 CC 23-17 (Aliphatic Compounds)
 Section cross-reference(s): 24, 25, 30
 IT 78-79-5, reactions 106-98-9, reactions 106-99-0, reactions 108-05-4, reactions 513-35-9 542-92-7, reactions 563-46-2 590-18-1 624-64-6
 R.I. RCT (Reactant); RACT (Reactant or reagent)
 (addition reaction of, with acetic acid, catalysts for)
 IT 105-87-3P 141-12-8P 542-10-9P 625-16-1P
 628-08-0P 637-27-4P 1191-16-8P 29297-48-1P
 54830-99-8P
 R.I. SPN (Synthetic Preparation); PREP (Preparation)
 (Preparation of)

L74 ANSWER 52 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1982:581684 HCAPLUS FULL-TEXT
 DOCUMENT NUMBER: 97:181684
 TITLE: Syntheses by sulfones. XXIII. Selectivity of the synthesis of allylic sulfones
 AUTHOR(S): Julia, Marc; Nél, Maurice; Righini, Anne; Uguen, Daniel
 CORPORATE SOURCE: Lab. Chim., Ec. Natl. Supér., Paris, 75231, Fr.
 SOURCE: Journal of Organometallic Chemistry (1982), 235(1), 113-20
 CODEN: JORCAL; ISSN: 0022-328X

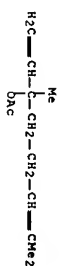
DOCUMENT TYPE: French
 LANGUAGE: CASREACT 97:181684
 OTHER SOURCE(S):
 ED Entered STN: 12 May 1984
 AB Pd complexes catalyzed the reaction of conjugated dienes with arenesulfonic acids or of allylic acetates with Na arenesulfonates. For example, treatment of isoprene with p-toluenesulfonic acid in the presence of (π-allyl)palladium chloride (I) or bis(dibenzylideneacetone)palladium and ligands PhP₃, P(C₆H₄Me-O)₃, P(OEt)₃, P(COCH₃)₂, or Ph₂PCl₂CH₂Ph₂ gave mainly Me₂C(SO₂CH₃Me-p)-CH:CH₂ along with small amts. of Me₂C:CH(CH₂)₂CO₂CH₃Me-p and other minor products. Treatment of Me₂C:CH(CH₂)₂CO₂CH₃Me-p with Na p-toluenesulfonate in the presence of I and PhP₃ gave 86% Me₂C:CH(CH₂)₂CO₂CH₃Me-p. Tertiary sulfones are favored under mild reaction conditions. The ligands also influence the reactivity. Arenesulfonic acids catalyzed the isomerization of secondary or tertiary allylic sulfones to primary sulfones.
 IT 105-87-3 115-95-7 141-12-8
 R.I. RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with sodium toluenesulfinate, catalytic)
 RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

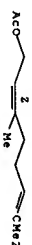


RN 115-95-7 HCAPLUS
 CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)

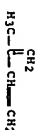


RN 141-12-8 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

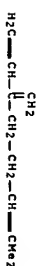
Double bond geometry as shown.



IT 78-79-5, reactions 123-35-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with toluenesulfonic acid, catalytic)
 RN 78-79-5 HCAPLUS
 CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)



RN 123-35-3 HCAPLUS
 CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



CC 23-17 (Aliphatic Compounds)
 Section cross-reference(s): 22, 25
 IT 105-87-3 115-95-7 141-12-8
 24509-88-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with sodium toluenesulfinate, catalytic)
 IT 78-79-5, reactions 123-35-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with toluenesulfonic acid, catalytic)

174 ANSWER 53 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1981:495775 HCAPLUS Full-text
 DOCUMENT NUMBER: 95:99775
 TITLE: Use of 1,3,5,5-tetramethyl-2-oxabicyclo[2.2.2]octane in augmenting or enhancing the aroma or taste of foods

INVENTOR(S):

Vock, Manfred H.; Vinals, Joaquin F.; Kivala, Jacob

PATENT ASSIGNEE(S): International Flavors and Fragrances Inc., USA
 U.S. 21 pp. Cont.-in-part of U.S. 4,195,099.

SOURCE:

DOCUMENT TYPE:

LANGUAGE:

PATENT INFORMATION:

PATENT NO.

US 4269862

US 4195099

US 4203947

US 4283576

US 4267067

US 4289705

US 4303725

US 4320771

US 4289705

US 4303725

US 4320771

US 4289705

US 4303725

PATENT NO. KIND DATE APPLICATION NO. DATE

US 4269862 A 19810526 US 1979-77539 1979

US 4195099 A 19800325 US 1978-953128 1978

US 4203947 A 19800520 US 1979-8925 1979

US 4283576 A 19810811 US 1979-100528 1979

US 4267067 A 19810512 US 1980-176093 1980

US 4289705 A 19810915 US 1980-176050 1980

US 4303725 A 19811201 US 1980-176092 1980

US 4320771 A 19820323 US 1980-176112 1980

US 4289705 A 19810915 US 1980-176050 1980

US 4303725 A 19811201 US 1980-176092 1980

US 4320771 A 19820323 US 1980-176112 1980

US 4289705 A 19810915 US 1980-176050 1980

US 4303725 A 19811201 US 1980-176092 1980

US 4320771 A 19820323 US 1980-176112 1980

US 4289705 A 19810915 US 1980-176050 1980

US 4303725 A 19811201 US 1980-176092 1980

US 4320771 A 19820323 US 1980-176112 1980

US 4289705 A 19810915 US 1980-176050 1980

US 4303725 A 19811201 US 1980-176092 1980

US 4320771 A 19820323 US 1980-176112 1980

US 4289705 A 19810915 US 1980-176050 1980

US 4303725 A 19811201 US 1980-176092 1980

US 4320771 A 19820323 US 1980-176112 1980

US 4289705 A 19810915 US 1980-176050 1980

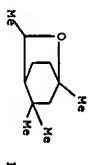
US 4303725 A 19811201 US 1980-176092 1980

US 4320771 A 19820323 US 1980-176112 1980

US 4289705 A 19810915 US 1980-176050 1980

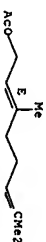
US 4303725 A 19811201 US 1980-176092 1980

US 1979-52334 A3 1979 0202
 <--
 US 1979-77539 A3 1979 0627
 <--
 US 1979-77539 A3 1979 0921
 <--
 ED Entered STN: 12 May 1984
 GI



AB 1,3,5,5-Tetramethyl-2-oxabicyclo[2.2.2]octane (I) [78474-70-1] is prepared and used to give a fresh or minty flavor to food, tobacco, pharmaceuticals, and other products. Thus, methyl oxide [141-79-7] in a suspension of AlCl₃ in MePh was reacted with isoprene [78-79-5] to yield 4-acetyl-1,3,3-trimethyl-1-cyclohexene [55695-36-8]. The latter was reduced with NaBH₄ to give 1,3,3-trimethyl-1-cyclohexene-4-ethanol [78474-71-2] which was reacted with iso-PrOH [67-63-0] and H₂SO₄ to yield I. A pleasant citrus nuance and sour effect when I was included at 200 ppm.

IT 105-87-3 141-12-8
 RL: BIOL (Biological study)
 RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)
 Double bond geometry as shown.

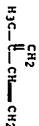


RN 141-12-8 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)
 Double bond geometry as shown.



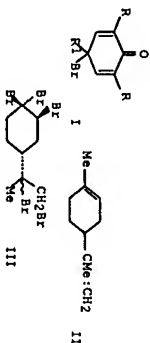
IT 78-79-5, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)

Reaction of, with methyl oxide)
 RN 78-79-5 HCAPLUS
 CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)



IC A231001-226
 INCL 426536000
 CC 17-2 (Foods)
 Section cross-reference(s): 62, 63
 IT Flavoring materials
 (tetramethyloxabicyclooctane)
 IT 75-07-0, biological studies 78-70-6 80-56-8 87-44-5
 92-52-4, biological studies 94-62-2 98-55-5 99-49-0
 99-86-5 105-87-3 110-89-4, biological studies
 118-71-8 120-57-0 121-32-4 123-11-5, biological studies 127-91-3 138-86-3 141-12-8 470-82-6
 495-91-0 555-10-2 586-62-9 1329-99-3 4674-50-4 5392-40-5
 14575-74-7 38049-26-2
 RL: BIOL (Biological study)
 IT 78-79-5, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with methyl oxide)

L74 ANSWER 54 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1980:568419 HCAPLUS Full-text
 DOCUMENT NUMBER: 93:168419
 TITLE: Cyclization of polyenes. Part 32. Selective bromination of polyenes by 2,4,4,6-tetrabromocyclohexa-2,5-dienone
 Kato, Tadahiro; Ichinohe, Isao
 Dep. Chem., Tohoku Univ., Sendai, 980 Japan
 Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1980), (5), 1051-6
 CODEN: JCPR84; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 93:168419
 ED Entered STN: 12 May 1984
 GI

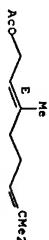


AB Geranyl cyanide reacted with the bromo ketones I (R = R₁ = Br, Cl; R = Br, R₁ = Me) to give a mixture of hexabromocyclohexa-2,5-dienone, CH₂:CMeBrCBr(CH₂)₂CMe:CHCH₂Br, and

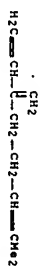
BrCH₂CMe:CH(CH₂)₂CMe:CHCH₂CH with the former predominating in yields of 98, 40, and 45%, resp. This mild selective bromination was extended to a range of polyenes using CTAB and I (R = R₁ = Br). E.g., the polyene II gave 87% III. The di- or tetrabromo products I are formed by sequential reactions.

- IT 105-87-3 123-35-3
 R₁: RCT (Reactant); RACT (Reactant or reagent)
 (bromination of, by tetrabromocyclohexadecene, selective)
 RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



- RN 123-35-3 HCAPLUS
 CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



- CC 30-10 (Terpenoids)
 Section cross-reference(s): 23, 24
 IT 100-42-5, reactions 105-87-3 110-83-8, reactions
 123-35-3 126-91-0 1189-09-9 4176-77-6 5989-27-5
 6485-40-1 21677-96-3 36237-68-0 42207-88-5

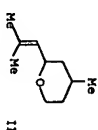
R₁: RCT (Reactant); RACT (Reactant or reagent)
 (bromination of, by tetrabromocyclohexadecene, selective)

- L74 ANSWER 55 OF 67 HCAPLUS COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 1980:495409 HCAPLUS Full-text
 DOCUMENT NUMBER: 93:95409

TITLE:
 The reaction of hypochlorous acid with olefins. A convenient synthesis of allylic chlorides

AUTHOR(S):
 Hegde, Shridhar G.; Vogel, Martin K.; Saddler, John; Hirano, Tanya; Rockwell, Ned; Haynes, Robert; Oliver, Michael; Molinsky, Joseph
 CORP. SOURCE: Dep. Chem., Purdue Univ., West Lafayette, IN, 47907, USA
 SOURCE: Tetrahedron Letters (1980), 21(5), 441-4
 CODEN: TETLEA; ISSN: 0040-4039

DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 12 May 1984

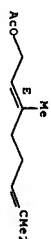


II

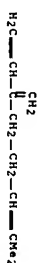
AB HOCl reacts with highly substituted olefins in CH₂Cl₂ to give allylic chlorides. E.g., Me₂C:CH(CH₂)₂CMe:CH(R = CHO, CO₂Me, CH₂OH, CH₂OMe) reacted with HOCl to give 60-80% CH₂:CMeCHCl(CH₂)₂CMe:CH(R (I). The utility of the reaction is illustrated by preparation of α-monoterpene and Rose oxide. Thus, sequential treatment of I (R = CHO, CO₂Me, CH₂OH) with Zn-TfP and H₂O gave CH₂:CMe(CH₂)₂CMe:CH(R, and sequential treatment of Me₂C:CH(CH₂)₂CMe(CH₂)₂OR (R = H, Ac) with HOCl, NaOH-ROH, and H₂SO₄ gave .appx. 50% Rose oxide (II).

- IT 105-87-3 123-35-3 150-84-5
 R₁: RCT (Reactant); RACT (Reactant or reagent)
 (chlorination of, by hypochlorous acid-methylene chloride)
 RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

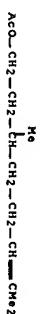
Double bond geometry as shown.



- RN 123-35-3 HCAPLUS
 CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



- RN 150-84-5 HCAPLUS
 CN 6-Octen-1-ol, 3,7-dimethyl-, 1-acetate (CA INDEX NAME)



- CC 30-10 (Terpenoids)
 Section cross-reference(s): 23
 IT 78-70-6 89-79-2 99-49-0 105-87-3 106-22-9
 106-24-1 106-25-2 123-35-3 141-27-5 150-84-5
 591-49-1 1189-09-9 1195-92-2 4602-84-0 7212-44-4
 13466-78-9 55298-92-5 56695-54-6 74514-15-1 74514-25-3
 R₁: RCT (Reactant); RACT (Reactant or reagent)
 (chlorination of, by hypochlorous acid-methylene chloride)

L74 ANSWER 56 OF 67 HCAPLUS COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 1979:509091 HCAPLUS Full-text
 DOCUMENT NUMBER: 91:108091
 TITLE:
 A facile functionalization of the isopropylidene terminus of isoprenoids. Application to the synthesis of terminal trans allylic alcohols
 AUTHOR(S): Masaki, Yukio; Hashimoto, Kenji; Kaji, Kenji
 CORP. SOURCE: Gifu Coll. Pharm., Gifu, Japan

SOURCE: Tetrahedron Letters (1978), (46), 4539-42

CODEN: TELFAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 12 May 1984

AB trans-PtCH₂CH₂CH:CH₂CH₂CH(R₁) (I; R₁ = CH₃) on addition reaction with PhSeCl, followed by dehydrochlorination in DMF (60°, 20 h) or silica gel treatment and dehydration, gave I (R = SP₃, R₁ = CH₃;CH₃) which on oxidation and treatment with (MeO)₃P gave I (R₁ = trans-C(CH₂OH)Me) stereospecifically [76% from I (R₁ = CH₃)]. Other terminal trans allylic alcs. were prepared (47-80%) from isoprenoids by similar functionalization of the isopropylidene terminus.

IT 105-87-3 115-95-7 123-35-3

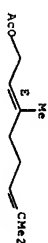
141-12-8 1191-16-8

RL: RCT (Reactant); RACT (Reactant or reagent)

RN 105-87-3 HCAPLUS

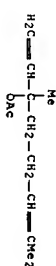
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 115-95-7 HCAPLUS

CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)



RN 123-35-3 HCAPLUS

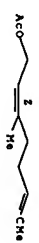
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



RN 141-12-8 HCAPLUS

CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.



RN 1191-16-8 HCAPLUS

CN 2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)

AcO-CH₂-CH=CH₂

CC 30-10 (Terpenoids)

Section cross-reference(s): 23

IT 105-87-3 115-95-7 123-35-3

141-12-8 556-82-1 1191-16-8 22089-60-7

52188-73-5 53254-60-7 55802-98-7 59632-99-4 68690-44-8

70473-30-2 70473-31-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(addition reaction of, with benzenesulfonyl chloride)

L74 ANSWER 57 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1978:7078 HCAPLUS Full-Text

DOCUMENT NUMBER: 88:7078

TITLE: Highly stereoselective synthesis of nerol and geraniol

AUTHOR(S): Juntao Takabe, Kunihiko Katagiri, Takao Tanaka,

Fac. Eng., Shizuoka Univ., Hamamatsu, Japan

Chemistry Letters (1977), (9), 1025-6

CODEN: CHMTAG; ISSN: 0366-7022

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 12 May 1984

AB Nerol was prepared stereoselectively by telomerization of isoprene in the presence of dialkylamine followed by treatment with ClCO₂Et, conversion of (2)-Me₂C=CHCH₂CH₂CH₂CH₂Cl to the acetate, and hydrolysis of the acetate. Geraniol was synthesized similarly via (E)-Me₂C=CHCH₂CH₂CH₂CH₂Cl from myrcene and p₂NH.

IT 105-87-3P 141-12-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

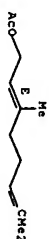
(Preparation); RACT (Reactant or reagent)

(Preparation and hydrolysis of)

RN 105-87-3 HCAPLUS

CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 141-12-8 HCAPLUS

CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.



IT 541-41-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with dialkyl(dimethyl)octadecylamine)

CC#CCCC=C(C)CCOC(=O)C

IT	123-35-3	RCT (Reactant); RACT (Reactant or reagent)
CN	1,6-octadiene, 7-methyl-3-methylene- (CA INDEX NAME)	(reaction with diethylamine in presence of sodium naphthalenide, diethylgeranylamine from)
RN	123-35-3	HCAPUS

$$\text{H}_2\text{C}=\text{CH}-\overset{\text{CH}_2}{\underset{|}{\text{C}}}-\text{CH}_2-\text{CH}_2-\text{CH}=\text{CH}_2$$

CC	30-10 (Terpenoids)
IT	105-87-3P 105-90-8P 106-29-6P 109-20-6P 2345-26-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RL: RCT (Reactant) ; RACT (Reactant or reagent)
(reaction with diethylamine in presence of sodium
naphthalenide, diethylgeranylamine from)

L74 ANSWER 60 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:74443 HCAPLUS Full-text
DOCUMENT NUMBER: 84:74443
TITLE: Terpenoid alcohols and acetates from the

AUTHOR(S): Kaal, T.; Laats, K.
CORPORATE SOURCE: Inst. Khim., Tallin, USSR
SOURCE: Eesti NSV Teaduste Akadeemia Toimetised

CODEN: EKEGAI; ISSN: 0424-6373

ED Entered S

AB Mixts. of terpene chlori

AB
Mixts. of terpine chlorides prepared by telomerization of isoprene with its hydrochlorides were saponified and the unreacted chlorides dehydrochlorinated with alic. KOH to give linaloal, Me2C:CHCH2CHCH(OH)CMe:CH2, Me2C:CHCH2CH2CH:O=CMeCH2OH, and a mixture of α -terpineol and m-menth-6-en-8-ol.

IT 80-26-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN	80-26-2	HCAPLUS
CN	3-Cyclohexene-1-methanol, $\alpha,\alpha,4$ -trimethyl-, 1-acetate (CA INDEX NAME)	

IT	78-79-5	reactions
	RL RCT (Reactant); RACT (Reactant or reagent)	
	(telomerization of, with its hydrochlorides, alcs. and acetates	
	from)	
RN	78-79-5	HCAPLUS
CN	1,3-Butadiene, 2-methyl-	(CA INDEX NAME)

$$\text{H}_3\text{C}-\overset{\text{CH}_2}{\underset{\text{CH}_2}{\text{C}}}-\text{CH}_2$$

CC	30-10 (Tepenooids)
IT	80-26-2P 25-49-04-1P 58336-04-2P
IT	Rt.: SPN (Synthetic preparation); PREP (Preparation) (Preparation of)
IT	78-79-5, reactions
	Rt.: RCT (Reactant); RACT (Reactant or reagent)
	(telomerization of, with its hydrochlorides, alcs. and acetates from)

174 ANSWER 61 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STNN
ACCESSION NUMBER: 1974:132720 HCAPLUS Full-text:
DOCUMENT NUMBER: 80:132720
TITLE: Reaction of amines with conjugated

AUTHOR(S): Fujita, T.; Suga, K.; Watanabe, S.
CORPORATE SOURCE: Fac. Eng., Chiba Univ., Chiba, Japan
SOURCE: Australian Journal of Chemistry (1977)

CODEN: AJCHAS; ISSN: 0004-9425

DOCUMENT TYPE: Journal
LANGUAGE: English

ED Entered STN: 12 May 1984

AB Reaction of a conjugated diene with EtCNH using Na naphthalenide in THF gave a mixture of β , γ -unsatd., amine. From mycene, *N,N*-diethyl-2-ethylidene-6-methylhept-5-enylamine, *N,N*-diethylmerylamine and *N,N*-diethylgeranylamine were obtained. Reaction of β , γ -unsatd. amines with Ac₂O gave a mixture of β , γ -unsatd., acetates. From *N,N*-diethylgeranylamine, a mixture of methyl acetate and geranyl acetate was obtained.

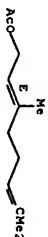
IT 105-87-3P 141-12-8P 1191-16-8P

RL: SPN (Synthetic

(preparation of)

RN	HCAPLUS	CA INDEX
CN	2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)-	(CA INDEX NAME)

Double bond geometry as shown.

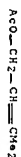


RN 141-12-8 HCAPLUS
CN 2,6-Octadiene-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

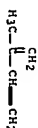
Double bond geometry as shown.



RN 1191-16-8 HCAPLUS
CN 2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)



IT 78-79-5, reactions 123-35-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(With amines, in presence of alkali naphthalenides)
RN 78-79-5 HCAPLUS
CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)



RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



CC 23-4 (Aliphatic Compounds)
Section cross-reference(s): 27, 28, 30
IT 105-87-3P 141-12-8P 688-92-6P

1191-16-8P 5300-21-0P 10229-36-4P 17734-30-4P
24509-88-4P 27973-92-8P 27973-95-1P 36794-55-5P
36794-56-6P 37857-39-9P 37857-40-2P 40137-00-6P
40267-43-4P 40267-47-8P 40267-48-9P 40267-53-6P
51930-65-5P 51930-66-6P 51930-67-7P 51930-68-8P
51930-69-9P 51930-70-2P 51930-72-4P 51930-73-5P
52027-04-0P 59313-90-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
IP: Preparation of

IT 78-79-5, reactions 123-35-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(With amines, in presence of alkali naphthalenides)

L74 ANSWER 62 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:26777 HCAPLUS Full-text
DOCUMENT NUMBER: 80:26777
TITLE: Unsaturated diesters

INVENTOR(S): Ono, Isao; Yanagihara, Tadshisa; Okada,
Hitkazu; Koga, Toshikuni
PATENT ASSIGNEE(S): Toyo Soda Manufg. Co., Ltd.
SOURCE: Jpn. Tokyoo Koho, 4 pp.
CODEN: JAKXAB
Patent
Japanese

DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 4802889	B	19730905	JP 1968-90547	1968
				1212

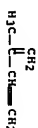
PRIORITY APPLN. INFO.:

JP 1968-90547
1968
1212

Entered STN: 12 May 1984

AB 2-Butene-1,4-diol esters acyclic or cyclic, with alkyl substituents or none, were obtained by reaction of conjugated dienes with carboxylic acids in the presence of Pd salts, transition metal salts, and alkali or alkali metal salts. Thus, 16.3 g butadiene, 100 g AcOH, 0.65 g Pd(OAc)₂, 15.0 g Cu(OAc)₂, and 10.9 g NaOAc was treated at 80° under 15 atm O for 3 hr to give 14.5 g 1,4-diacetoxy-2-butene. Similarly prepared were 1,4-diacetoxy-2-methyl-2-butene, 3,5-dipropionyloxy-1-cyclopentene, and 3,6-diformyloxy-1-cyclohexene.

IT 78-79-5, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
78-79-5 HCAPLUS
CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)



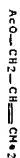
IT 127-09-3
RL: CAT (Catalyst use); USES (Uses)
(Catalysts, with cupric and palladium acetates, for addition of acetic acid to butadienes)
RN 127-09-3 HCAPLUS
CN Acetic acid, sodium salt (1:1) (CA INDEX NAME)



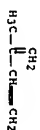
Na

IC C07C
CC 23-17 (Aliphatic Compounds)
Section cross-reference(s): 24
IT Esters, preparation
RL: PREP (Preparation)
(unsatd. di-)

RI: RCT (Reactant); RACT (Reactant or reagent)
(terpenoids from isoprene and)
RN 1191-16-8 HCAPLUS
CN 2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)



IT 78-79-5, reactions
RI: RCT (Reactant); RACT (Reactant or reagent)
(terpenoids from prenyl acetate and)
RN 78-79-5 HCAPLUS
CN 1,3-Butadiene, 2-methyl-, (CA INDEX NAME)



CC 30 (Terpenoids)
IT 80-26-2P 16109-44-2P 24604-60-2P 25905-14-0P
33843-18-4P 33843-20-8P
RI: SPN (Synthetic preparation); PREP (preparation)
(preparation of)
IT 1191-16-8
RI: RCT (Reactant); RACT (Reactant or reagent)
(terpenoids from isoprene and)
IT 78-79-5, reactions
RI: RCT (Reactant); RACT (Reactant or reagent)
(terpenoids from prenyl acetate and)

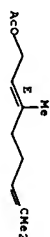
174 ANSWER 65 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970-531138 HCAPLUS Full-text
DOCUMENT NUMBER: 73121138
TITLE: Complexes of terpenes with transition metals.
III. Dimerization by means of
tetrakis(triphenylphosphine)palladium
Dunne, K.; McQuillan, Francis J.
Dep. Org. Chem., Univ. Newcastle-upon-Tyne,
Newcastle-upon-Tyne, UK
Journal of the Chemical Society [Section] C:
Organic (1970), (16), 2203-6
CODEN: JSOQAX; ISSN: 0022-4952
Journal

AUTHOR(S):
CORPORATE SOURCE:
SOURCE:

DOCUMENT TYPE:

LANGUAGE: English
ED Entered STN: 12 May 1984
AB Tetrakis(triphenylphosphine)palladium dimethanes neolidyl acetate, and 1-
vinylcyclohexyl acetate to linear dimers, and myrcene to a monocyclic dimeric product.
IT 105-87-3 123-35-3
RI: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with palladium phosphine complexes)
RN 105-87-3 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



CC 30 (Terpenoids)
IT 105-87-3 123-35-3 2306-78-7,
1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, acetate 6318-49-6
RI: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with palladium phosphine complexes)

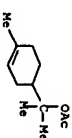
174 ANSWER 66 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970-133026 HCAPLUS Full-text
DOCUMENT NUMBER: 72133026
TITLE: Terpenyl acetates
INVENTOR(S): Clark, John Colin
PATENT ASSIGNEE(S): A. Boake, Roberts and Co. Ltd.
SOURCE: Brit., 3 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1172516		19691203	GB 1965-51023	1965 1201

ED Entered STN: 12 May 1984

AB The esters of linalol, geraniol, and nerol were prepared from myrcene. Thus, a mixture of 50 lb 80% myrcene, 250 lb AcOH, and 0.5 lb tert-butylcatechol was stirred in an inert atmosphere at 110-20° 36 hr to give 10 lb acetate esters, containing 55% geranyl and nerol acetates, 15% myrcenyl acetates, and 12% α-terpinyl acetate.
IT 80-26-2P 105-87-3P 141-12-0P
RI: SPN (Synthetic preparation); PREP (preparation)
(preparation of)

RN 80-26-2 HCAPLUS
CN 3-Cyclohexene-1-methanol, α,α,4-trimethyl-, 1-acetate
(CA INDEX NAME)



RN 105-87-3 HCAPLUS

IT 78-79-5, reactions 542-92-7 592-57-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 IT 127-09-3 (addition to, of carboxylic acids, catalysts for)
 RL: CAT (Catalyst use); USES (Uses)
 (catalysts, with cupric and palladium acetates, for addition of acetic acid to butadienes)

L74 ANSWER 63 OF 67 HCAPLUS COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 1973:418895 HCAPLUS Full-text
 DOCUMENT NUMBER: 79:18895
 TITLE: Terpene alcohols and their acetates and formates

INVENTOR(S): Fukui, Kenichi; Kagitani, Tsutomu; Yamanka, Toru

PATENT ASSIGNEE(S): Takasago Perfumery Co., Ltd.
 SOURCE: Jpn. Tokyo Kono, 2 pp.
 CODEN: JAXXAD

DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

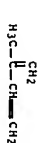
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 48010766	B	19730407	JP 1969-93950	1969 1125

PRIORITY APPL. INFO.:
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 JP 1969-93950
 1969
1125

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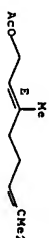
ED Entered STN: 12 May 1984
 AB Terpene alcs. and their acetates and formates were prepared by dimerization of isoprene in liquid CO₂ by catalytic use of 85% H₃PO₄ or 70% H₂SO₄ in the presence of H₂O, AcOH, or HCO₂H. E.g., a mixture of isoprene 34, AcOH 50, 85% H₃PO₄ 24, and CO₂ 100 g was kept 1 hr at 17° to give, after steam distillation, 11.2 g distillate containing geranyl (main), linalyl, myrcenyl, and terpenyl acetates. Geranyl, linalyl, and myrcenyl formates and geraniol, linalol, and myrcenol were also obtained.

IT 78-79-5, (Reaction); RACT (Reactant or reagent)
 RL: RCT (Reactant); RACT (Reactant or reagent)
 RN 78-79-5 HCAPLUS
 CN 1,3-butadiene, 2-methyl- (CA INDEX NAME)

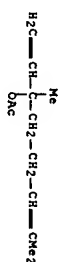


IT 105-87-3P 115-95-7P
 RL: PREP (Preparation)
 (from dimerization of isoprene)
 RN 105-87-3 HCAPLUS
 CN 2,6-octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 115-95-7 HCAPLUS
 CN 1,6-octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)



IC COTC: B01J
 CC 30-10 (Terpenoids)
 IT 78-79-5, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 IT 105-87-3P 115-95-7P 118-39-4P 13461-20-6P
 RL: PREP (Preparation)
 (from dimerization of isoprene)

L74 ANSWER 64 OF 67 HCAPLUS COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 1971:529947 HCAPLUS Full-text
 DOCUMENT NUMBER: 75:129947
 TITLE: Syntheses of terpenoids by telomerization. V. Cationic telomerization of isoprene with prenyl acetate

AUTHOR(S): Juntao

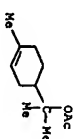
CORPORATE SOURCE: Fac. Eng., Shizuoka Univ., Hamamatsu, Japan
 SOURCE: Kogyo Kagaku Zasshi (1971), 74(6), 1162-4
 CODEN: KKGZAT; ISSN: 0368-5462

DOCUMENT TYPE: Journal
 LANGUAGE: Japanese

ED Entered STN: 12 May 1984
 GI For diagram(s), see printed CA Issue.

AB A mixture of isoprene 3,4, prenyl acetate (I) 6.4, and EtOAc 6.4 g was mixed dropwise during 10 min with a solution containing 0.9 g BF₃·Et₂O in 1.5 g EtOAc and heated 1 hr at 20°. The structures of the telomers obtained (II-VII) were determined by IR and NMR spectroscopy. The reaction of I in the presence of acidic catalysts was also discussed. Based on the exptl. results, a reaction mechanism was proposed.

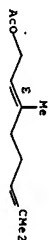
IT 80-26-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (Preparation of)
 RN 80-26-2 HCAPLUS
 CN 3-cyclohexene-1-methanol, α,α,4-trimethyl-, 1-acetate (CA INDEX NAME)



IT 1191-16-8

CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z) - (CA INDEX NAME)

Double bond geometry as shown.

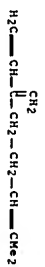


RN 141-12-8 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z) - (CA INDEX NAME)

Double bond geometry as shown.



IT 123-35-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acetic acid)
RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



IC C07C
CC 30 (Terpenoids)
IT 80-26-2P 105-87-3P 141-12-8P
1118-39-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 123-35-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acetic acid)

L74 ANSWER 67 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1967:76161 HCAPLUS Full-text
DOCUMENT NUMBER: 66:76161
TITLE: Reaction gas chromatography. II.
Dehydrogenation of monoterpene compounds on
platinum-alumina catalyst

AUTHOR(S): Mizrahi, Isaac; Nigam, Ishwar C.
CORPORATE SOURCE: Food Drug Directorate, Ottawa, Can.
SOURCE: Journal of Chromatography (1966),
25(2), 230-41
CODEN: JOCRAM; ISSN: 0021-9673

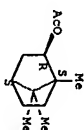
DOCUMENT TYPE: English
LANGUAGE: English
ED Entered STN: 12 May 1984
AB cf. CA 66, 75418P. Dehydrogenation of 42 monoterpenes was investigated using a reactor packed with 5% Pt on Al2O3. Products obtained were analyzed by gas chromatography on 3 instruments using a thermal conductivity detector, and a H flame ionization detector.

Exptl. data correlated with the structures of the parent compds. Mechanisms of dehydrogenations and isomerizations involved were discussed.

IT 76-49-3 105-87-3 115-95-7
123-35-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydrogenation of, chromatog. and)

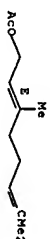
RN 76-49-3 HCAPLUS
CN Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, 2-acetate,
(1R,2S,4R)-tel- (CA INDEX NAME)

Relative stereochemistry.

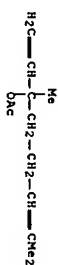


RN 105-87-3 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z) - (CA INDEX NAME)

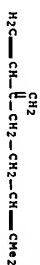
Double bond geometry as shown.



RN 115-95-7 HCAPLUS
CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)



RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



CC 30 (Terpenes)
IT 76-49-3 78-70-6 79-92-5 80-56-8, reactions 89-48-5
98-55-5 99-82-1 99-83-2 99-86-5 105-86-2 105-87-3
106-22-9 106-24-1 115-95-7 115-99-1 123-35-3
127-91-3 138-86-3 491-05-4 498-15-7 500-00-5 507-70-0
586-62-9 586-67-4 1134-95-8 1197-07-5 1490-04-6
1632-73-1 3387-41-5 7786-67-6 13877-91-3 29563-98-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydrogenation of, chromatog. and)

-> d his nofile

(FILE 'HOME' ENTERED AT 10:23:49 ON 16 MAY 2007)

FILE 'HCAPLUS' ENTERED AT 10:24:09 ON 16 MAY 2007

E US20070055076/PN

L1 1 SEA ABB=ON PLU=ON US20070055076/PN

D ALL

SEL RN

FILE 'REGISTRY' ENTERED AT 10:25:28 ON 16 MAY 2007

L2 35 SEA ABB=ON PLU=ON (100-66-3/BI OR 105-87-3/BI OR

105-90-8/BI OR 105-91-9/BI OR 106-24-1/BI OR 106-25-2/B

1 OR 106-42-3/BI OR 107-92-6/BI OR 108-21-4/BI OR

108-86-3/BI OR 108-90-7/BI OR 108-94-1/BI OR 109-20-6/B

1 OR 1191-16-8/BI OR 123-35-3/BI OR 123-86-4/BI OR

127-08-2/BI OR 127-09-3/BI OR 137-40-6/BI OR 138-86-3/B

1 OR 141-12-8/BI OR 142-96-1/BI OR 157258-67-8/BI OR

19559-59-2/BI OR 3915-83-1/BI OR 503-74-2/BI OR

5392-40-5/BI OR 556-82-1/BI OR 64-19-7/BI OR 78-79-5/BI

OR 78-93-3/BI OR 79-09-4/BI OR 79-31-2/BI OR 80-26-2/B

1 OR 851785-97-2/BI)

L3 19 SEA ABB=ON PLU=ON L2 AND ?ACID?/CNS

D SCAN

L4 1 SEA ABB=ON PLU=ON 123-35-3/RN

D SCAN

L5 1 SEA ABB=ON PLU=ON 78-79-5/RN

D IDE

L6 1 SEA ABB=ON PLU=ON 1191-16-8/RN

D IDE

L7 1 SEA ABB=ON PLU=ON 105-87-3/RN

D SCAN

L8 1 SEA ABB=ON PLU=ON 141-12-8/RN

D IDE

L9 11 SEA ABB=ON PLU=ON L2 AND ?ACETATE?/CNS

D IDE

FILE 'STINGUIDE' ENTERED AT 10:44:21 ON 16 MAY 2007

FILE 'CASREACT' ENTERED AT 10:50:09 ON 16 MAY 2007

L10 1 SEA ABB=ON PLU=ON 123-35-3/RCT(L) (105-87-3/PRO OR

141-12-8/PRO)

D SCAN

L11 2 SEA ABB=ON PLU=ON 78-79-5/RCT(L) (1191-16-8/PRO

D SCAN

E ESTER/CT

E ESTERS/CT

L12 23 SEA ABB=ON PLU=ON 64-19-7/RCT(L) (123-35-3/RCT OR

78-79-5/RCT)

D SCAN

L13 STR 123-35-3

L14 36 SEA SSS SAM L13 (448 REACTIONS)

L15 789 SEA SSS FUL L13 (11229 REACTIONS)

SAV L15 LA0307CRCT/A

E ESTERS/CT

L16 7147 SEA ABB=ON PLU=ON ESTERS+PFT OLD /NT/CT

D SCAN

L17 7 SEA ABB=ON PLU=ON L15 AND L16

D SCAN

D QUE

L18 SAV L17 LA0307CRCTA/A
 L19 STR L13
 L20 6 SEA SUB-L15 SSS SAM L18 (28 REACTIONS)
 L21 D SCAN
 L22 88 SEA SUB-L15 SSS FUL L18 (708 REACTIONS)
 L23 SAV L20 LA0307CRCTB/A
 L24 STR L18
 L25 1 SEA SUB-L15 SSS SAM L21 (7 REACTIONS)
 L26 D SCAN
 L27 5 SEA SUB-L15 SSS FUL L21 (16 REACTIONS)
 L28 SAV L23 LA0307CRCTC/A
 L29 STR L21
 L30 1 SEA SUB-L15 SSS SAM L24 (7 REACTIONS)
 L31 D SCAN
 L32 7 SEA SUB-L15 SSS FUL L24 (38 REACTIONS)
 L33 D SCAN
 L34 SAV L26 LA0307CRCTD/A
 L35 STR L27 LA0307CRCTE/A
 L36 34 SEA ABB-ON PLU-ON (L10 OR L11 OR L12) OR L17 OR L23
 L37 OR L26
 L38 43 SEA ABB-ON PLU-ON BABLER JAMES?/AU
 L39 3 SEA ABB-ON PLU-ON L27 AND L28
 L40 SAV L29 LA0307CRCTIN/A
 L41 31 SEA ABB-ON PLU-ON L27 NOT L29
 L42 FILE 'HCAPIUS' ENTERED AT 12:06:06 ON 16 MAY 2007
 L43 QUE ABB-ON PLU-ON PY<2004 OR PRY<2004 OR AY<2004 OR
 L44 MY<2004 OR REVIEW/DI
 L45 1 SEA ABB-ON PLU-ON L1 AND L31
 L46 D SCAN
 L47 FILE 'CASREACT' ENTERED AT 12:07:53 ON 16 MAY 2007
 L48 25 SEA ABB-ON PLU-ON L30 AND L31
 L49 3 SEA ABB-ON PLU-ON L29 AND L31
 L50 FILE 'HCAPIUS' ENTERED AT 12:08:48 ON 16 MAY 2007
 L51 D SCAN L1
 L52 619 SEA ABB-ON PLU-ON L4/RAC
 L53 5537 SEA ABB-ON PLU-ON L5/RAC
 L54 86 SEA ABB-ON PLU-ON L6/P
 L55 347 SEA ABB-ON PLU-ON L7/P
 L56 D 1-2 KWIC
 L57 144 SEA ABB-ON PLU-ON L8/P
 L58 D KWIC
 L59 D 1-2 L36 KWIC
 L60 0 SEA ABB-ON PLU-ON L36(L1)L37
 L61 12 SEA ABB-ON PLU-ON L36 AND L37
 L62 0 SEA ABB-ON PLU-ON L35(L1) (L38 OR L39)
 L63 10 SEA ABB-ON PLU-ON L35 AND (L38 OR L39)
 L64 20 SEA ABB-ON PLU-ON (L40 OR L41 OR L42 OR L43)
 L65 34845 SEA ABB-ON PLU-ON L9
 L66 70 SEA ABB-ON PLU-ON (L35 OR L36) AND L45
 L67 4036 SEA ABB-ON PLU-ON L9/RAC
 L68 50 SEA ABB-ON PLU-ON (L35 OR L36) AND L47
 L69 9 SEA ABB-ON PLU-ON L48 AND L44
 L70 E ESTERS/CT
 L71 QUE ABB-ON PLU-ON ESTERS+PFT,OLD,NTI/CT
 L72 70 SEA ABB-ON PLU-ON L44 OR L46 OR (L48 OR L49)
 L73 47 SEA ABB-ON PLU-ON L51 AND L50
 L74 E VITAMINS/CT
 L75 QUE ABB-ON PLU-ON VITAMINS+PFT,OLD,NT/CT
 L76 E FLAVOR/CT
 L77 E FLAVORS/CT
 L78 E FLAVORING/CT
 L79 QUE ABB-ON PLU-ON FLAVOR+PFT,OLD,NT/CT

L55 3 SEA ABB-ON PLU-ON L51 AND (L53 OR L54)
 L56 D SCAN
 L57 D SCAN L1
 L58 E "DIETARY SUPPLEMENTS"/CT
 L59 QUE ABB-ON PLU-ON "DIETARY SUPPLEMENTS"+PFT,OLD,NT/CT
 L60 QUE ABB-ON PLU-ON "FLAVORING MATERIALS"+PFT,OLD,NT/CT
 L61 "ODOR AND ODOROUS SUBSTANCES"+PFT,O
 L62 LD,NT/CT
 L63 45 SEA ABB-ON PLU-ON L52 AND L31
 L64 SAV L59 LA0307HCE/A
 L65 43 SEA ABB-ON PLU-ON L28
 L66 D QUE
 L67 43 SEA ABB-ON PLU-ON L60 AND L31
 L68 QUE ABB-ON PLU-ON VITAM? OR ODOR? OR SMELL? OR
 L69 PERFUM? OR SUPPLEMENT? OR FLAVOR?
 L70 4 SEA ABB-ON PLU-ON L61 AND L62
 L71 4 SEA ABB-ON PLU-ON L61 AND (L53 OR L56 OR L57 OR L58)
 L72 D QUE
 L73 5 SEA ABB-ON PLU-ON L51 AND (L53 OR L56 OR L57 OR L58)
 L74 45 SEA ABB-ON PLU-ON L55 OR L59 OR L65
 L75 45 SEA ABB-ON PLU-ON L66 AND L31
 L76 SAV L67 LA0307HCE/A
 L77 6 SEA ABB-ON PLU-ON L63 OR L64
 L78 13 SEA ABB-ON PLU-ON L61 AND L50
 L79 17 SEA ABB-ON PLU-ON L68 OR L69
 L80 SAV L70 LA0307HCEIN/A
 L81 D QUE L67
 L82 43 SEA ABB-ON PLU-ON L67 NOT L70
 L83 D QUE L34
 L84 D QUE L33
 L85 FILE 'CASREACT' ENTERED AT 12:45:36 ON 16 MAY 2007
 L86 D QUE L33
 L87 FILE 'STINGUIDE' ENTERED AT 12:46:03 ON 16 MAY 2007
 L88 FILE 'MEDLINE, BIOSIS, DRUGU, EMBASE' ENTERED AT 12:46:36 ON 16
 L89 MAY 2007
 L90 4 SEA ABB-ON PLU-ON L28
 L91 D 1-4 TI
 L92 SAV L72 LA0307IN/A
 L93 FILE 'STINGUIDE' ENTERED AT 12:47:53 ON 16 MAY 2007
 L94 D QUE L34
 L95 D QUE L70
 L96 D QUE L72
 L97 FILE 'CASREACT, HCAPIUS, BIOSIS' ENTERED AT 12:49:46 ON 16 MAY
 L98 2007
 L99 19 DUP REM L34 L70 L72 (5 DUPLICATES REMOVED)
 L100 ANSWERS '1-3' FROM FILE CASREACT
 L101 ANSWERS '4-18' FROM FILE HCAPIUS
 L102 ANSWER '19' FROM FILE BIOSIS
 L103 FILE 'CASREACT' ENTERED AT 12:51:20 ON 16 MAY 2007
 L104 FILE 'CASREACT, HCAPIUS, BIOSIS' ENTERED AT 12:57:01 ON 16 MAY
 L105 2007
 L106 D L73 1-19 1818 ABS
 L107 FILE 'CASREACT' ENTERED AT 12:57:02 ON 16 MAY 2007

SN 10/564307 Page 139 of 139 STIC STN SEARCH 5/17/2007

FILE 'REGISTRY' ENTERED AT 12:57:42 ON 16 MAY 2007

D L4 IDE
D L5 IDE
D L6 IDE
D L7 IDE
D L8 IDE

FILE 'STNGUIDE' ENTERED AT 12:59:34 ON 16 MAY 2007

D QUE STAT L33
D QUE STAT L71

L74 FILE 'CASREACT, HCAPLUS' ENTERED AT 13:00:44 ON 16 MAY 2007
67 DUP REM L33 L71 (1 DUPLICATE REMOVED)

ANSWERS '1-25' FROM FILE CASREACT
ANSWERS '26-67' FROM FILE HCAPLUS

D L74 1-25 IBIB ABS FHIT
D L74 26-67 IBIB ED ABS HITSTR HITIND